STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 168070

TO: Tamthom Truong
Location: REM/5B19/5C18
Art Unit: 1624
Wednesday, October 19, 2005
Case Serial Number: 09/835523

From: John DiNatale
Location: Biotech-Chem Library
REM-1B65
Phone: (571)272-2557

john.dinatale@uspto.gov

Search Notes

Examiner Truong,

See attached results.

If you have any questions about this search feel free to contact me at any time.

Thank you for using STIC search services!

John DiNatale
Technical Information Specialist
STIC Biotech/Chem Library
(571)272-2557

STIC SEARCH RESULTS FEEDBACK FORM

Biotech-Chem Library

Questions about the scope or the results of the search? Contact ***the searcher or contact***:

Mary Hale, Information Branch Supervisor
Remsen Bldg. 01 D86
571-272-2507

Voluntary Results Feedback Form

- *I am an examiner in Workgroup:* ☐ *Example: 1610*
- *Relevant prior art **found**, search results used as follows:*
  - ☐ 102 rejection
  - ☐ 103 rejection
  - ☐ Cited as being of interest.
  - ☐ Helped examiner better understand the invention.
  - ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
  (journal articles, conference proceedings, new product announcements etc.)

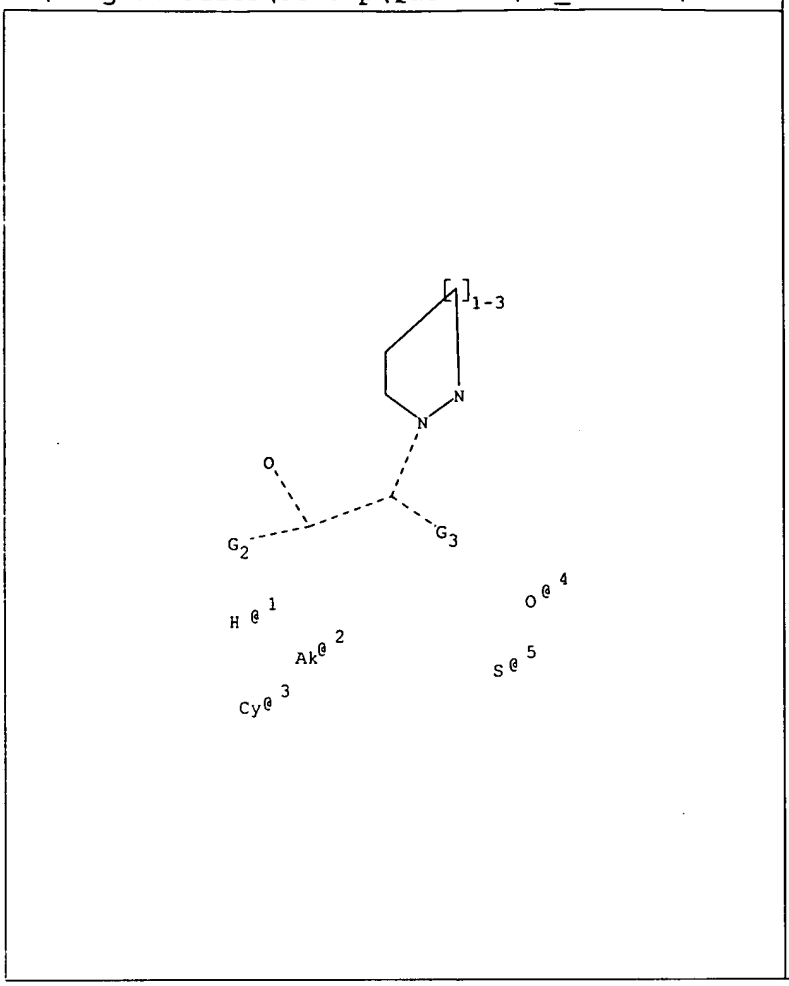
- *Relevant prior art **not found**:*
  - ☐ Results verified the lack of relevant prior art (helped determine patentability).
  - ☐ Results were not useful in determining patentability or understanding the invention.

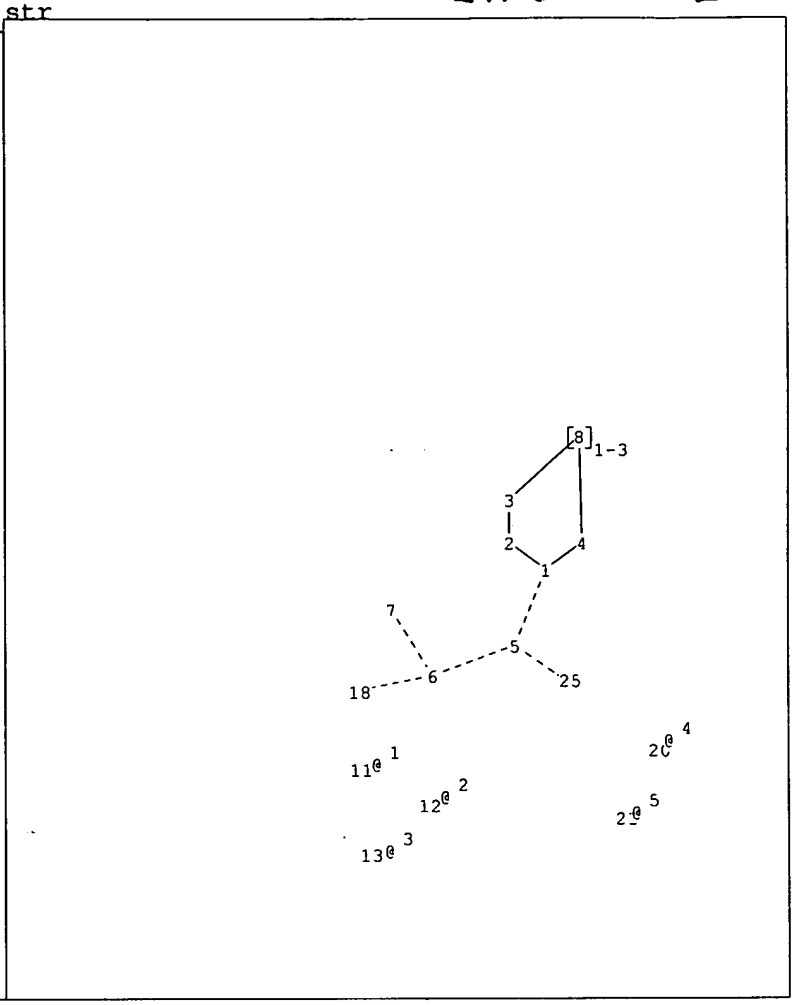
Comments:

Drop off or send completed forms to STIC-Biotech-Chem Library, Remsen Bldg.

C:\Program Files\Stnexp\Queries\09_835523\tru-a.str

structure "L1"





chain nodes :
5 6 7 11 12 13 18 20 21 25
ring nodes :
1 2 3 4 8
chain bonds :
1-5 5-6 5-25 6-7 6-18
ring bonds :
1-2 1-4 2-3 3-8 4-8
exact/norm bonds :
1-2 1-4 1-5 2-3 3-8 4-8 5-6 5-25 6-7 6-18

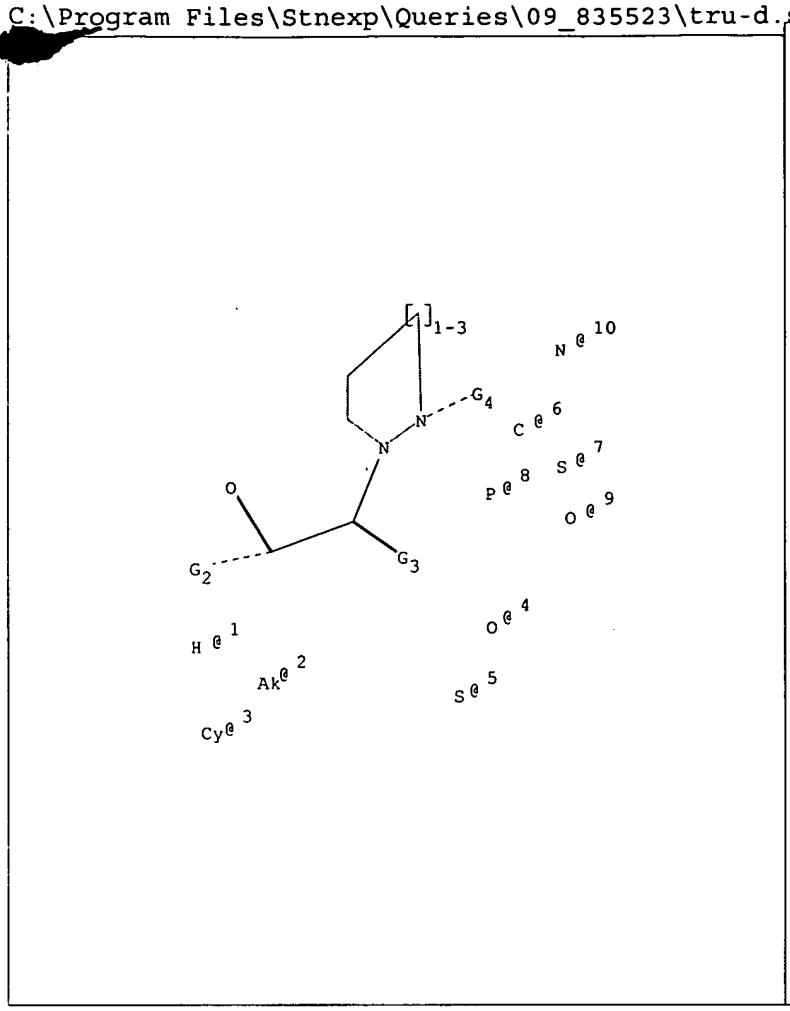
G2:[*1],[*2],[*3]

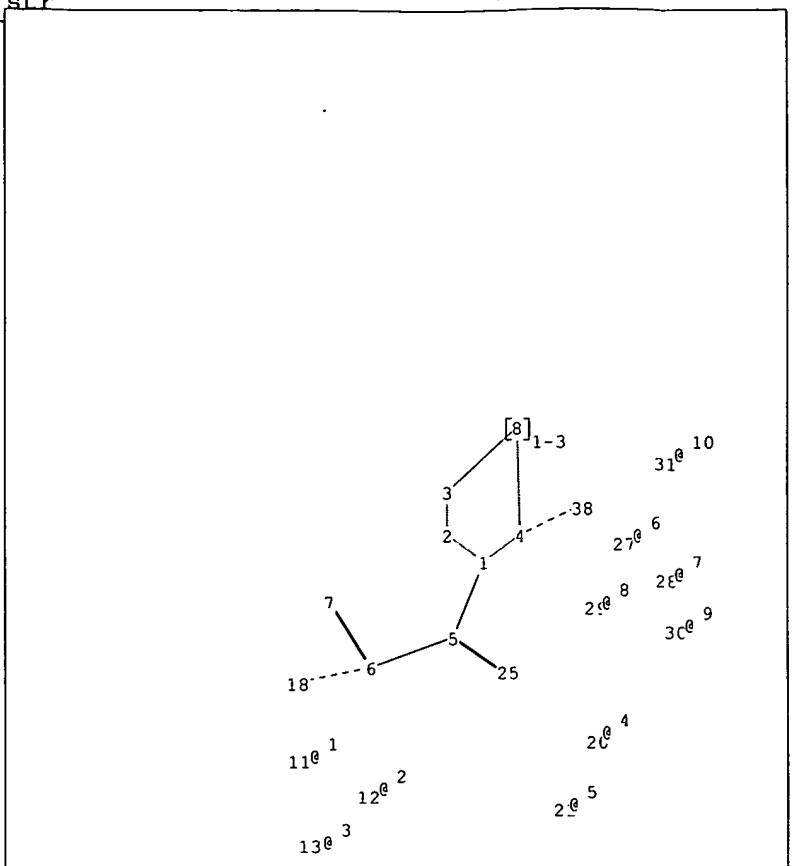
G3:[*4],[*5]

Connectivity :
5:3 E exact RC ring/chain 6:3 X maximum RC ring/chain 7:1 E exact RC ring/chain
20:1 E exact RC ring/chain 21:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:CLASS 6:CLASS 7:CLASS 8:Atom 11:CLASS 12:CLASS
13:Atom 18:CLASS 20:CLASS 21:CLASS 25:CLASS

C:\Program Files\Stnexp\Queries\09_835523\tru-d.str

structure "L21"





chain nodes :
5 6 7 11 12 13 18 20 21 25 38
ring nodes :
1 2 3 4 8
ring/chain nodes :
27 28 29 30 31
chain bonds :
1-5 4-38 5-6 5-25 6-7 6-18
ring bonds :
1-2 1-4 2-3 3-8 4-8
exact/norm bonds :
1-2 1-4 1-5 4-8 4-38 5-25 6-7 6-18
exact bonds :
2-3 3-8 5-6
isolated ring systems :
containing 1 :

G2:[*1],[*2],[*3]

G3:[*4],[*5]

G4:[*6],[*7],[*8],[*9],[*10]

Connectivity :
5:3 E exact RC ring/chain 6:3 X maximum RC ring/chain 7:1 E exact RC ring/chain
20:1 E exact RC ring/chain 21:1 E exact RC ring/chain
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:CLASS 6:CLASS 7:CLASS 8:Atom 11:CLASS 12:CLASS
13:Atom 18:CLASS 20:CLASS 21:CLASS 25:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS 38:CLASS

C:\Program Files\Stnexp\Queries\09_835523\tru-e.str

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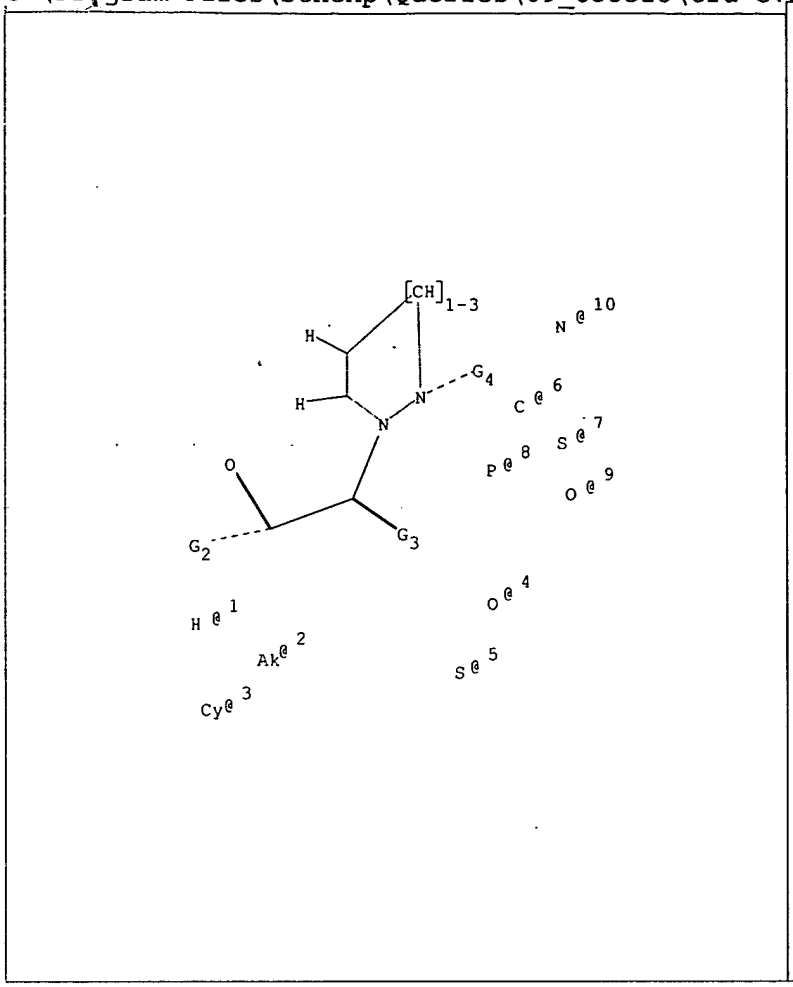

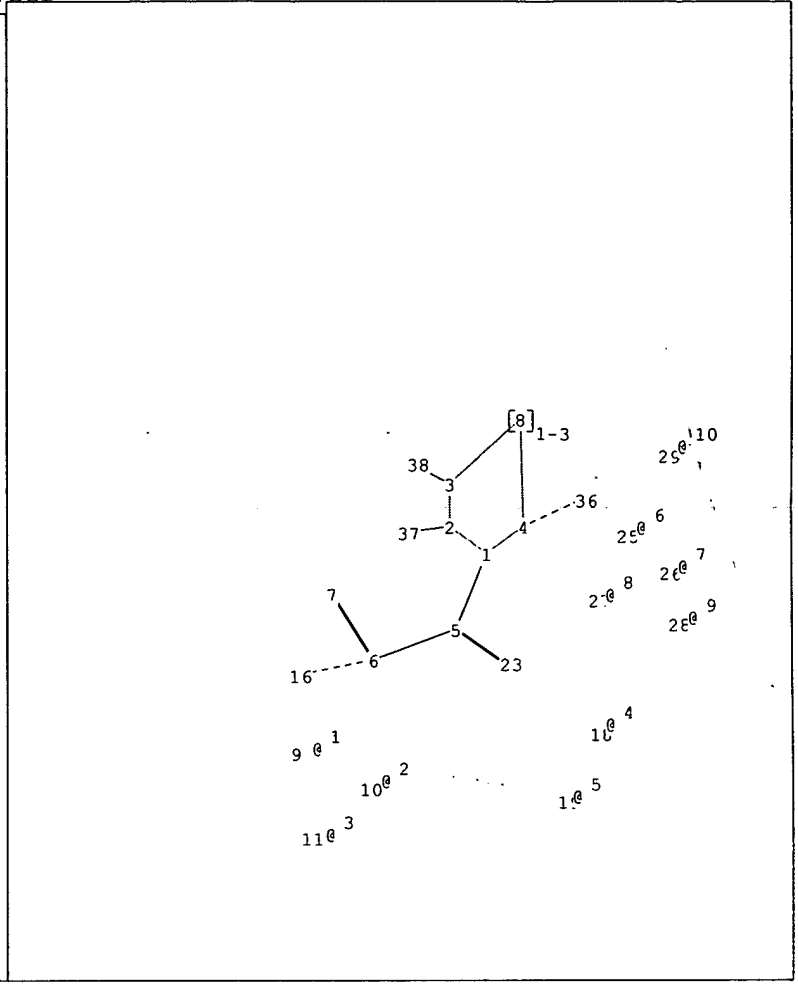

chain nodes :
5 6 7 9 10 11 16 18 19 23 36 37 38
ring nodes :
1 2 3 4 8
ring/chain nodes :
25 26 27 28 29
chain bonds :
1-5 2-37 3-38 4-36 5-6 5-23 6-7 6-16
ring bonds :
1-2 1-4 2-3 3-8 4-8
exact/norm bonds :
1-2 1-4 1-5 4-8 4-36 5-23 6-7 6-16
exact bonds :
2-3 2-37 3-8 3-38 5-6
isolated ring systems :
containing 1 :

G2:[*1],[*2],[*3]

G3:[*4],[*5]

G4:[*6],[*7],[*8],[*9],[*10]

Connectivity :
5:3 E exact RC ring/chain 6:3 X maximum RC ring/chain 7:1 E exact RC ring/chain
18:1 E exact RC ring/chain 19:1 E exact RC ring/chain
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:CLASS 6:CLASS 7:CLASS 8:Atom 9:CLASS 10:CLASS
11:Atom 16:CLASS 18:CLASS 19:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS
29:CLASS 36:CLASS 37:CLASS 38:CLASS

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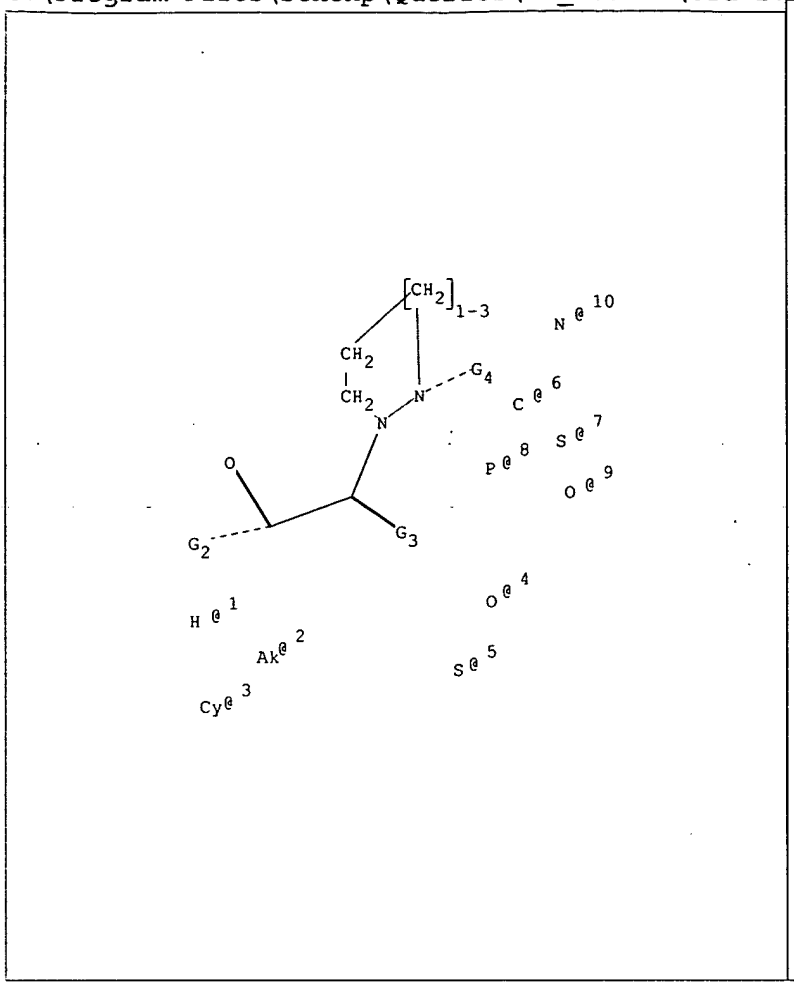

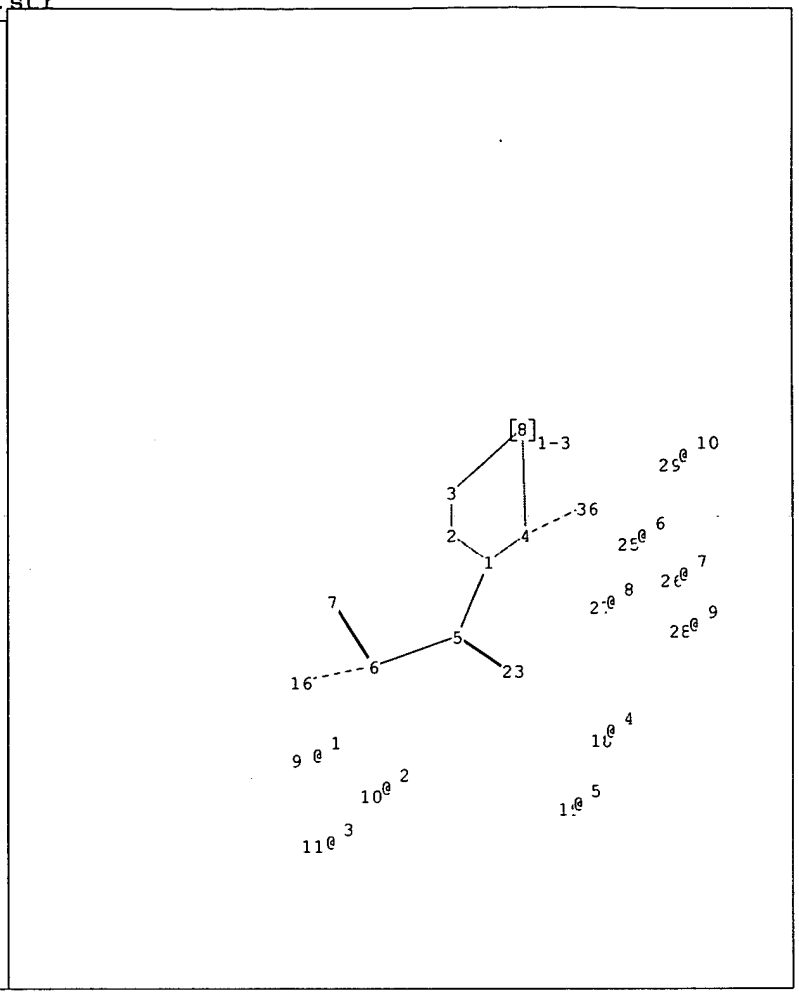

chain nodes :
5 6 7 9 10 11 16 18 19 23 36
ring nodes :
1 2 3 4 8
ring/chain nodes :
25 26 27 28 29
chain bonds :
1-5 4-36 5-6 5-23 6-7 6-16
ring bonds :
1-2 1-4 2-3 3-8 4-8
exact/norm bonds :
1-4 1-5 4-36 5-23 6-7 6-16
exact bonds :
1-2 2-3 3-8 4-8 5-6
isolated ring systems :
containing 1 :

G2:[*1],[*2],[*3]

G3:[*4],[*5]

G4:[*6],[*7],[*8],[*9],[*10]

Connectivity :
5:3 E exact RC ring/chain 6:3 X maximum RC ring/chain 7:1 E exact RC ring/chain
18:1 E exact RC ring/chain 19:1 E exact RC ring/chain
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:CLASS 6:CLASS 7:CLASS 8:Atom 9:CLASS 10:CLASS
11:Atom 16:CLASS 18:CLASS 19:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS
29:CLASS 36:CLASS

CAPlus (21 ~~hits~~ references) – broadest structure

Truong 09_835523 10/19/2005

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* available and contains the CA role and document type information.     *
*                                                                       *
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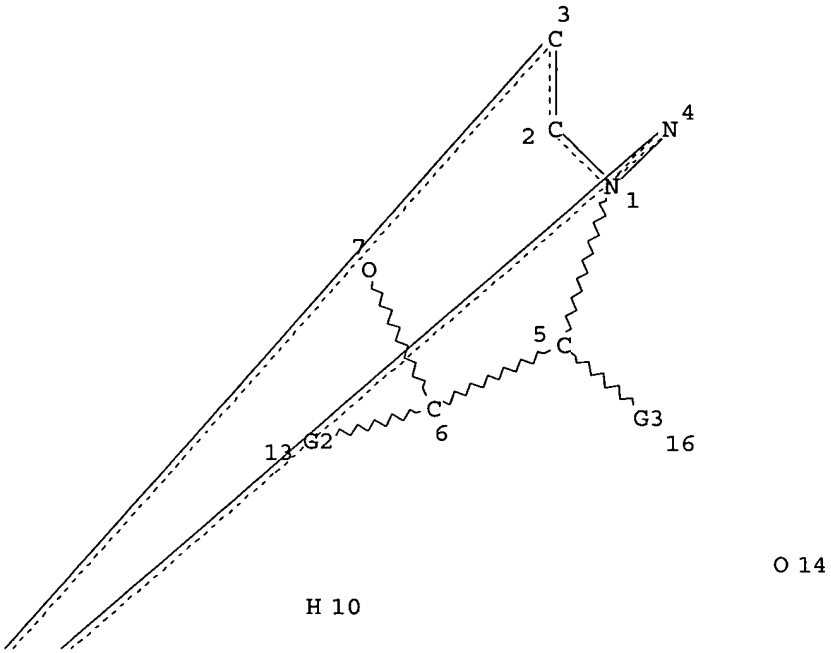
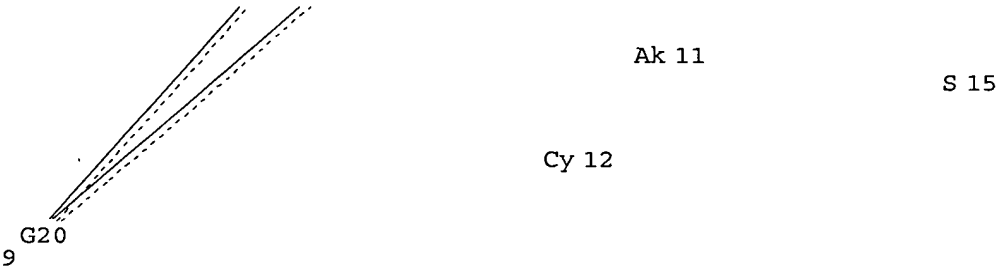
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d stat que L11
L1 STR



Page 1-A



Page 2-A
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VAR G3=14/15
REP G20=(1-3) 8-4 8-3
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NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS R AT 3
NSPEC IS R AT 4
NSPEC IS C AT 5

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NSPEC   IS C      AT   6
NSPEC   IS C      AT   7
NSPEC   IS R      AT   8
NSPEC   IS R      AT   9
NSPEC   IS C      AT  10
NSPEC   IS C      AT  11
NSPEC   IS C      AT  12
NSPEC   IS C      AT  13
NSPEC   IS C      AT  14
NSPEC   IS C      AT  15
NSPEC   IS C      AT  16
CONNECT IS E3  RC AT   5
CONNECT IS X3  RC AT   6
CONNECT IS E1  RC AT   7
CONNECT IS E1  RC AT  14
CONNECT IS E1  RC AT  15
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT   5  6  7 10 11 14 15
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  16

STEREO ATTRIBUTES: NONE
L10           76 SEA FILE=REGISTRY SSS FUL L1
L11           21 SEA FILE=CAPLUS ABB=ON  PLU=ON  L10


=> d ibib abs hitstr L11 1-21

L11  ANSWER 1 OF 21  CAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         2004:1013373  CAPLUS
DOCUMENT NUMBER:          142:134510
TITLE:                    An efficient diastereoselective glyoxylate-ene
                          reaction using N-glyoxyloyl camphorpyrazolidinone as
                          an enophile
AUTHOR(S):                Pan, Jia-Fu; Venkatesham, Uppala; Chen, Kwunmin
CORPORATE SOURCE:         Department of Chemistry, National Taiwan Normal
                          University, Taipei, 116, Taiwan
SOURCE:                   Tetrahedron Letters (2004), 45(51), 9345-9347
                          CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER:                Elsevier B.V.
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
OTHER SOURCE(S):          CASREACT 142:134510
GI
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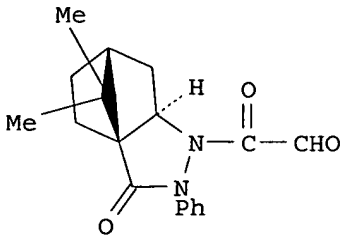
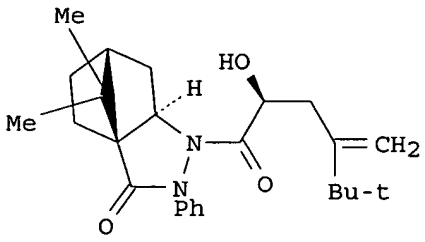


I



II

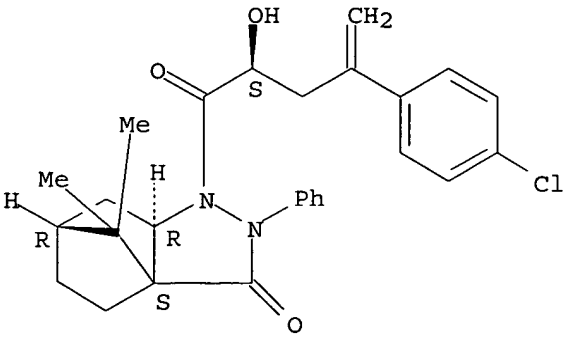
AB The diastereoselective glyoxylate-ene reaction of N-glyoxyloyl camphorpyrazolidinone with various alkenes in the presence of Lewis acid is described. The required (3aS,6R,7aR)-1-(1,2-dioxoethyl)hexahydro-8,8-dimethyl-2-phenyl-3a,6-methano-3aH-indazol-3(2H)-one (I) can be prepared from camphorpyrazolidinone (no data). The corresponding α-hydroxy carbonyls were generally obtained in moderate to high chemical yields (64-87%) and with high levels of diastereoselectivities (up to 94% de). The predominance of products with the (S) absolute configuration at the newly formed stereogenic center was established by single crystal X-ray anal. and the importance of stereochem. induction is discussed. The trifluoromethanesulfonic acid scandium(3+) salt-catalyzed ene reaction of I with 2,4,4-trimethyl-1-pentene gave a chiral α-hydroxy-γ-alkenyl carbonyl compound (II). The crystal and mol. structures of II were determined

IT **825619-71-4P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of chiral hexahydro[(chlorophenyl)(hydroxy)(methylene)(oxo)alkyl]di(methyl)(phenyl)-3a,6-methano-3aH-indazol-3(2H)-one and study of its crystal and mol. structures)

RN 825619-71-4 CAPLUS

CN 3a,6-Methano-3aH-indazol-3(2H)-one, 1-[(2S)-4-(4-chlorophenyl)-2-hydroxy-1-oxo-4-pentenyl]hexahydro-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



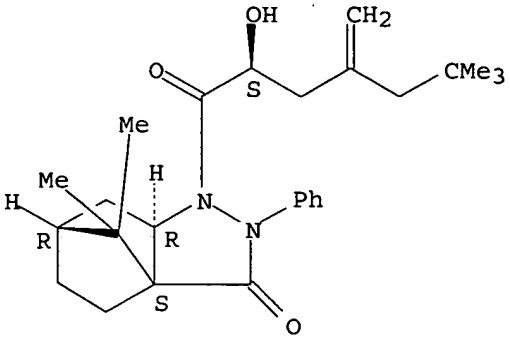
IT **825619-59-8P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of chiral hexahydro[(hydroxy)(methylene)(oxo)hexyl]di(methyl)(phenyl)-3a,6-methano-3aH-indazol-3(2H)-one and study of its crystal and mol. structures)

RN 825619-59-8 CAPLUS

CN 3a,6-Methano-3aH-indazol-3(2H)-one, hexahydro-1-[(2S)-2-hydroxy-6,6-

dimethyl-4-methylene-1-oxoheptyl]-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

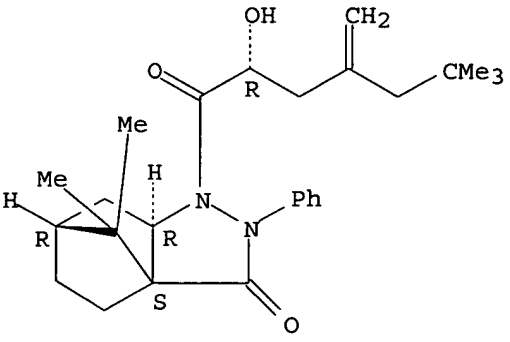


IT **825619-60-1P 825619-61-2P 825619-62-3P**
825619-63-4P 825619-64-5P 825619-65-6P
825619-66-7P 825619-67-8P 825619-68-9P
825619-69-0P 825619-70-3P 825619-72-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of chiral α-hydroxy-γ-alkenyl carbonyl compound by Lewis acid-catalyzed asym. ene reaction using (dioxoethyl)hexahydrodi(methyl)(phenyl)-3a,6-methano-3aH-indazol-3(2H)-one (chiral auxiliary) and alkene as starting materials)

RN 825619-60-1 CAPLUS

CN 3a,6-Methano-3aH-indazol-3(2H)-one, hexahydro-1-[(2R)-2-hydroxy-6,6-dimethyl-4-methylene-1-oxoheptyl]-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)-(9CI) (CA INDEX NAME)

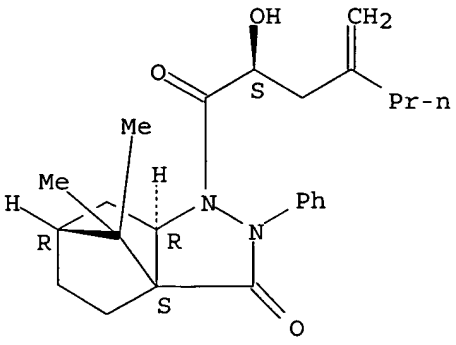
Absolute stereochemistry.



RN 825619-61-2 CAPLUS

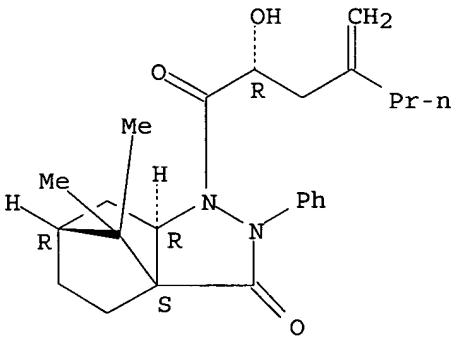
CN 3a,6-Methano-3aH-indazol-3(2H)-one, hexahydro-1-[(2S)-2-hydroxy-4-methylene-1-oxoheptyl]-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



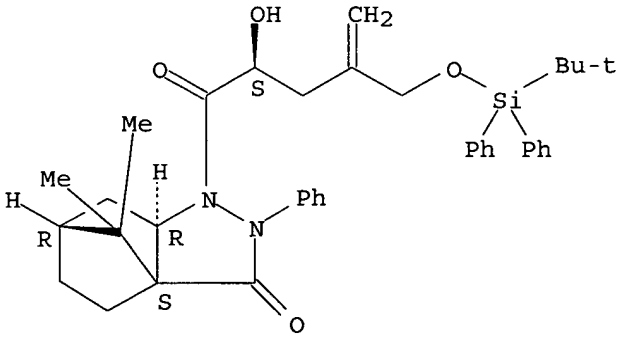
RN 825619-62-3 CAPLUS
CN 3a,6-Methano-3aH-indazol-3(2H)-one, hexahydro-1-[(2R)-2-hydroxy-4-methylene-1-oxoheptyl]-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 825619-63-4 CAPLUS
CN 3a,6-Methano-3aH-indazol-3(2H)-one, 1-[(2S)-4-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-2-hydroxy-1-oxo-4-pentenyl]hexahydro-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

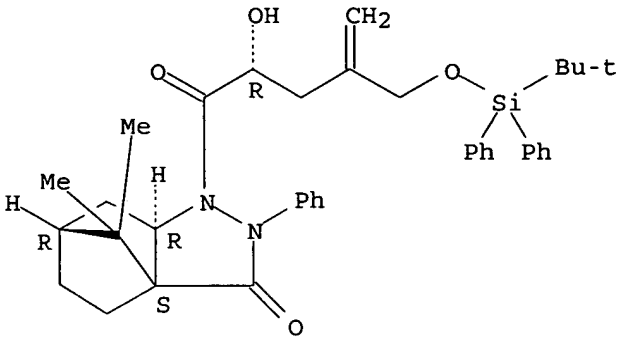
Absolute stereochemistry.



RN 825619-64-5 CAPLUS
CN 3a,6-Methano-3aH-indazol-3(2H)-one, 1-[(2R)-4-[[[(1,1-

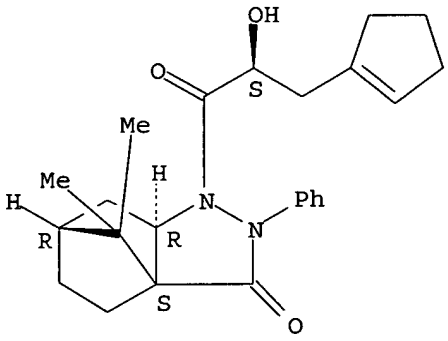
dimethylethyl)diphenylsilyl]oxy]methyl]-2-hydroxy-1-oxo-4-pentenyl]hexahydro-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



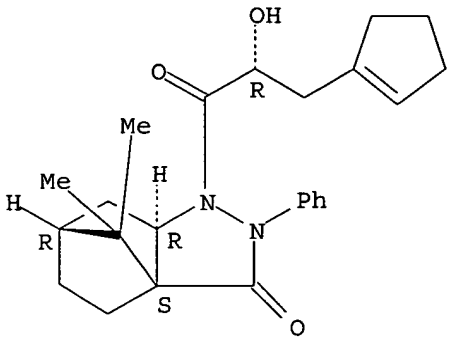
RN 825619-65-6 CAPLUS
CN 3a,6-Methano-3aH-indazol-3(2H)-one, 1-[(2S)-3-(1-cyclopenten-1-yl)-2-hydroxy-1-oxopropyl]hexahydro-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



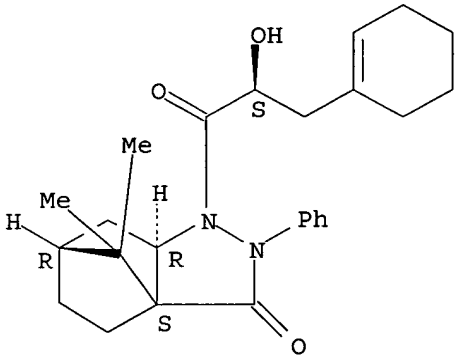
RN 825619-66-7 CAPLUS
CN 3a,6-Methano-3aH-indazol-3(2H)-one, 1-[(2R)-3-(1-cyclopenten-1-yl)-2-hydroxy-1-oxopropyl]hexahydro-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



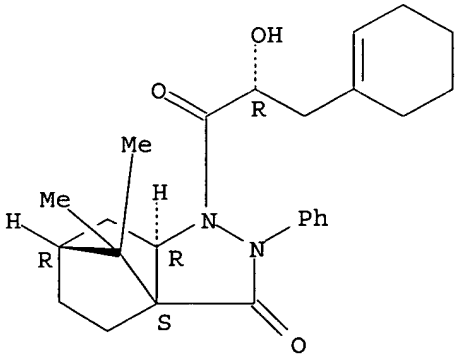
RN 825619-67-8 CAPLUS
CN 3a,6-Methano-3aH-indazol-3(2H)-one, 1-[(2S)-3-(1-cyclohexen-1-yl)-2-hydroxy-1-oxopropyl]hexahydro-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 825619-68-9 CAPLUS
CN 3a,6-Methano-3aH-indazol-3(2H)-one, 1-[(2R)-3-(1-cyclohexen-1-yl)-2-hydroxy-1-oxopropyl]hexahydro-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

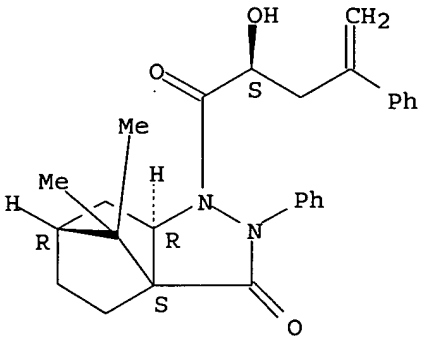
Absolute stereochemistry.



RN 825619-69-0 CAPLUS

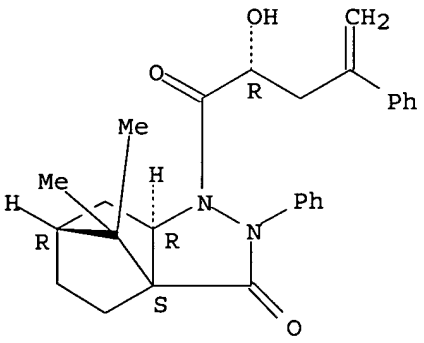
CN 3a,6-Methano-3aH-indazol-3(2H)-one, hexahydro-1-[(2S)-2-hydroxy-1-oxo-4-phenyl-4-pentenyl]-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



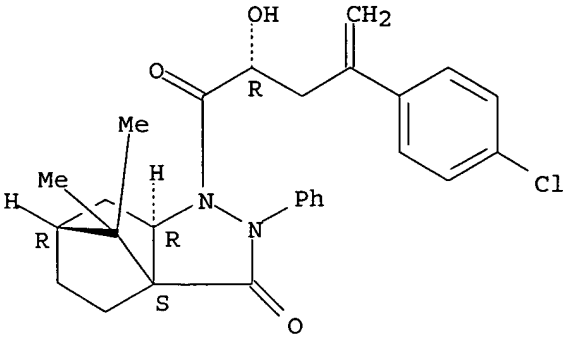
RN 825619-70-3 CAPLUS
CN 3a,6-Methano-3aH-indazol-3(2H)-one, hexahydro-1-[(2R)-2-hydroxy-1-oxo-4-phenyl-4-pentenyl]-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



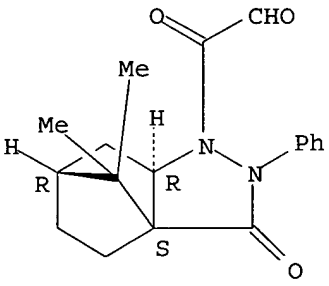
RN 825619-72-5 CAPLUS
CN 3a,6-Methano-3aH-indazol-3(2H)-one, 1-[(2R)-4-(4-chlorophenyl)-2-hydroxy-1-oxo-4-pentenyl]hexahydro-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



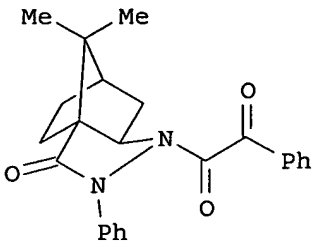
IT **682806-82-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of chiral α-hydroxy-γ-alkenyl carbonyl compds. by stereoselective ene reaction using (dioxoethyl)hexahydrodi(methyl)(phenyl)-3a,6-methano-3aH-indazol-3(2H)-one (chiral auxiliary) and alkenes as starting materials)
RN 682806-82-2 CAPLUS
CN 3a,6-Methano-3aH-indazole, octahydro-8,8-dimethyl-3-oxo-1-(oxoacetyl)-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

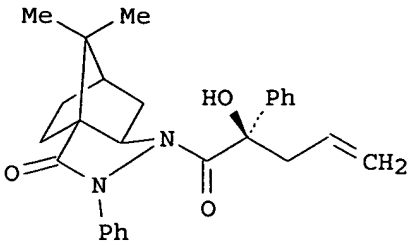


REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:580874 CAPLUS
DOCUMENT NUMBER: 141:260619
TITLE: Lewis acid mediated diastereoselective allylation of camphorpyrazolidinone derived α-ketoamides
AUTHOR(S): Wang, Shy-Guey; Tsai, Huei Ru; Chen, Kwunmin
CORPORATE SOURCE: Department of Chemistry, National Taiwan Normal University, Taipei, Taiwan
SOURCE: Tetrahedron Letters (2004), 45(32), 6183-6185
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:260619
GI



I



II

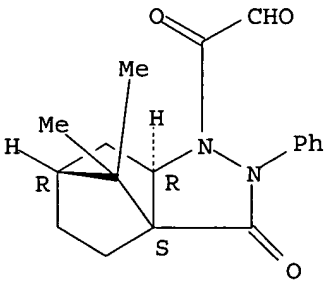
AB Diastereoselective allylation of camphorpyrazolidinone derived α-ketoamides, e.g., I, was examined using allyltributyltin in the presence of various Lewis acids. The corresponding optically enriched quaternary α-hydroxy carbonyls, e.g., II, were obtained in reasonable to excellent material yields (51-95%) and with practical levels of stereoselectivity (up to >95% de) when a stoichiometric amount of Sn(OTf)2 was used. The stereochem. induction is discussed.

IT **682806-82-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereoselective preparation of allyl(hydroxy)alkylcamphorpyrazolidinones via Lewis acid-catalyzed diastereoselective allylation of camphorpyrazolidinone derived α-ketoamides)

RN 682806-82-2 CAPLUS

CN 3a,6-Methano-3aH-indazole, octahydro-8,8-dimethyl-3-oxo-1-(oxoacetyl)-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

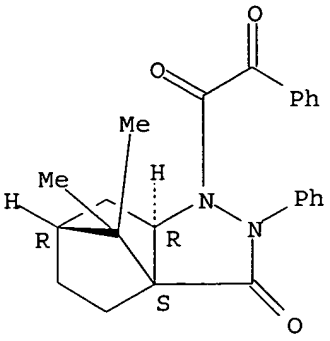


IT **756499-83-9P 756499-85-1P 756499-86-2P**
756499-87-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation of allyl(hydroxy)alkylcamphorpyrazolidinones via Lewis acid-catalyzed diastereoselective allylation of camphorpyrazolidinone derived α-ketoamides)

RN 756499-83-9 CAPLUS

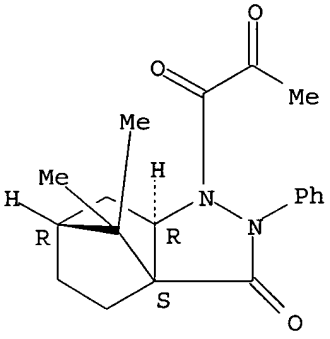
CN 3a,6-Methano-3aH-indazol-3(2H)-one, hexahydro-8,8-dimethyl-1-(oxophenylacetyl)-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



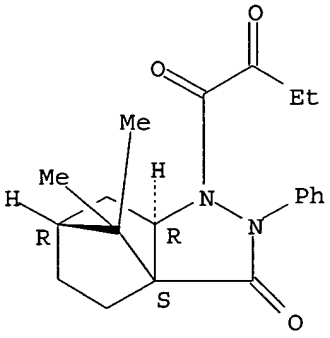
RN 756499-85-1 CAPLUS
CN 3a,6-Methano-3aH-indazol-3(2H)-one, 1-(1,2-dioxopropyl)hexahydro-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



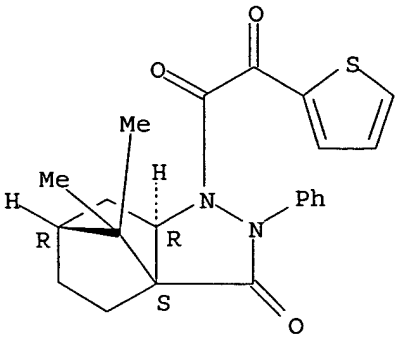
RN 756499-86-2 CAPLUS
CN 3a,6-Methano-3aH-indazol-3(2H)-one, 1-(1,2-dioxobutyl)hexahydro-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 756499-87-3 CAPLUS
CN 3a,6-Methano-3aH-indazol-3(2H)-one, hexahydro-8,8-dimethyl-1-(oxo-2-thienylacetyl)-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

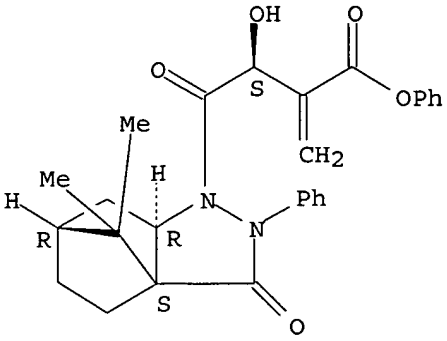
L11 ANSWER 3 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:170903 CAPLUS
DOCUMENT NUMBER: 140:357253
TITLE: Diastereoselective Baylis-Hillman reaction using N-glyoxyloyl camphorpyrazolidinone as an electrophile. Synthesis of optically pure 2-hydroxy-3-methylene succinic acid derivative
AUTHOR(S): Pan, Jia-Fu; Chen, Kwunmin
CORPORATE SOURCE: Department of Chemistry, National Taiwan Normal University, Taipei, 116, Taiwan
SOURCE: Tetrahedron Letters (2004), 45(12), 2541-2543
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The camphorpyrazolidinone derived N-glyoxylate was efficiently prepared and used as an electrophile in the Baylis-Hillman reaction under classical DABCO catalyzed conditions. The corresponding 2-hydroxy-3-methylene succinic acid derivative was generally obtained with excellent diastereoselectivity and moderate chemical yields (51-75%).

IT **682806-85-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(absolute configuration; preparation of optically pure 2-hydroxy-3-methylene succinic acid derivative by diastereoselective Baylis-Hillman reaction of N-glyoxyloyl camphorpyrazolidinone electrophile with α,β-unsatd. carbonyls/nitrile)

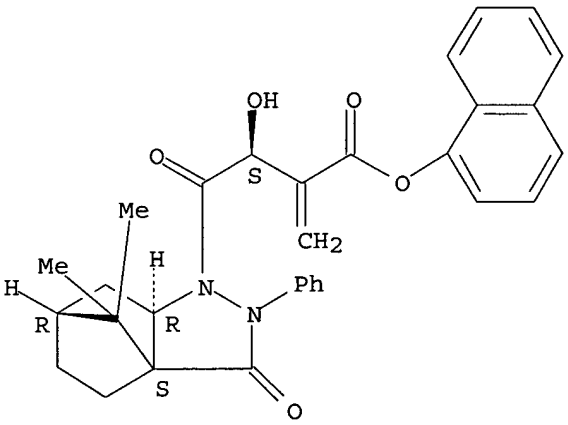
RN 682806-85-5 CAPLUS
CN 3a,6-Methano-3aH-indazole-1(4H)-butanoic acid, hexahydro-β-hydroxy-8,8-dimethyl-α-methylene-γ,3-dioxo-2-phenyl-, phenyl ester, (βS,3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



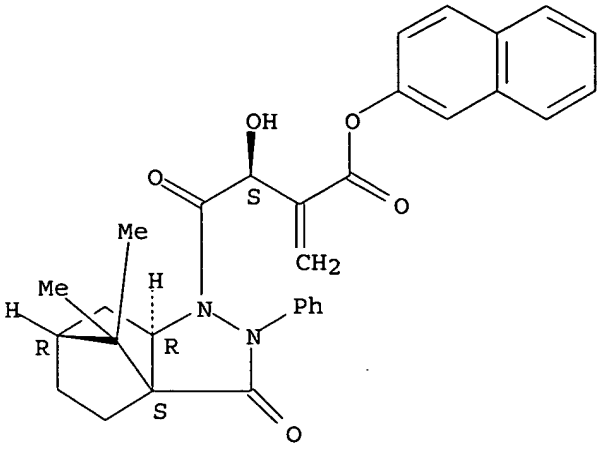
IT **682806-83-3P 682806-84-4P 682806-86-6P**
682806-87-7P 682806-88-8P 682806-89-9P
682806-90-2P 682806-91-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(absolute configuration; preparation of optically pure 2-hydroxy-3-methylene succinic acid derivative by diastereoselective Baylis-Hillman reaction of N-glyoxyloyl camphorpyrazolidinone electrophile with α,β-unsatd. carbonyls/nitrile)
RN 682806-83-3 CAPLUS
CN 3a,6-Methano-3aH-indazole-1(4H)-butanoic acid, hexahydro-β-hydroxy-8,8-dimethyl-α-methylene-γ,3-dioxo-2-phenyl-, 1-naphthalenyl ester, (βS,3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



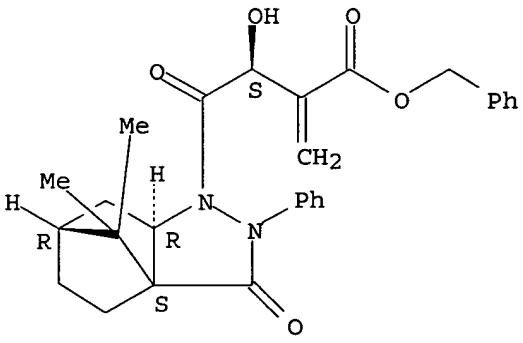
RN 682806-84-4 CAPLUS
CN 3a,6-Methano-3aH-indazole-1(4H)-butanoic acid, hexahydro-β-hydroxy-8,8-dimethyl-α-methylene-γ,3-dioxo-2-phenyl-, 2-naphthalenyl ester, (βS,3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



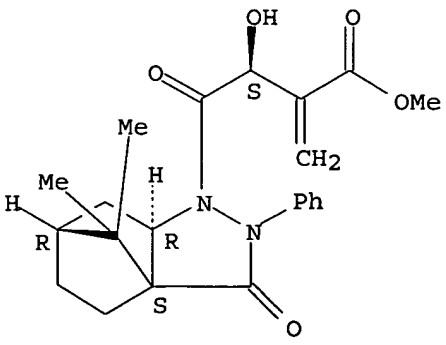
RN 682806-86-6 CAPLUS
CN 3a,6-Methano-3aH-indazole-1(4H)-butanoic acid, hexahydro-β-hydroxy-8,8-dimethyl-α-methylene-γ,3-dioxo-2-phenyl-, phenylmethyl ester, (βS,3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



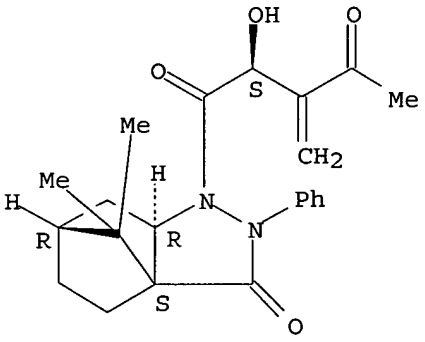
RN 682806-87-7 CAPLUS
CN 3a,6-Methano-3aH-indazole-1(4H)-butanoic acid, hexahydro-β-hydroxy-8,8-dimethyl-α-methylene-γ,3-dioxo-2-phenyl-, methyl ester, (βS,3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



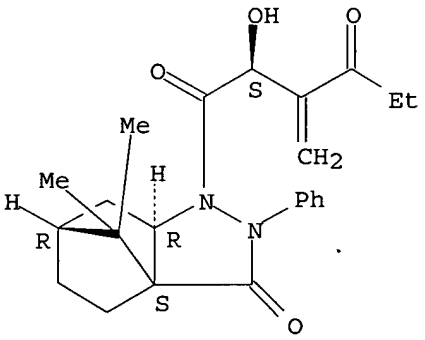
RN 682806-88-8 CAPLUS
CN 3a,6-Methano-3aH-indazol-3(2H)-one, hexahydro-1-[(2S)-2-hydroxy-3-methylene-1,4-dioxopentyl]-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



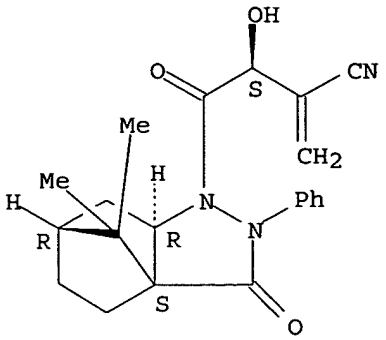
RN 682806-89-9 CAPLUS
CN 3a,6-Methano-3aH-indazol-3(2H)-one, hexahydro-1-[(2S)-2-hydroxy-3-methylene-1,4-dioxohexyl]-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



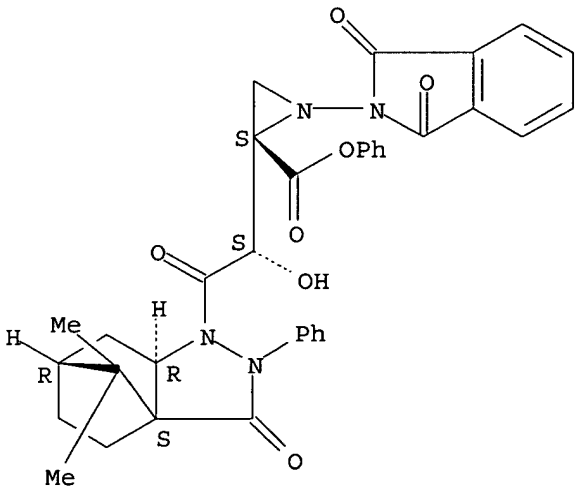
RN 682806-90-2 CAPLUS
CN 3a,6-Methano-3aH-indazol-3(2H)-one, 1-[(2S)-3-cyano-2-hydroxy-1-oxo-3-butenyl]hexahydro-8,8-dimethyl-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



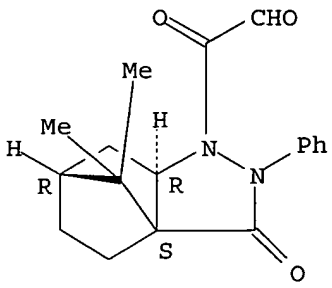
RN 682806-91-3 CAPLUS
CN 2-Aziridinecarboxylic acid, 1-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-2-[(1S)-1-hydroxy-2-[(3aS,6R,7aR)-hexahydro-8,8-dimethyl-3-oxo-2-phenyl-3a,6-methano-3aH-indazol-1(4H)-yl]-2-oxoethyl]-, phenyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **682806-82-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(electrophile; preparation of optically pure 2-hydroxy-3-methylene succinic acid derivative by diastereoselective Baylis-Hillman reaction of N-glyoxyloyl camphorpyrazolidinone electrophile with α,β-unsatd. carbonyls/nitrile)
RN 682806-82-2 CAPLUS
CN 3a,6-Methano-3aH-indazole, octahydro-8,8-dimethyl-3-oxo-1-(oxoacetyl)-2-phenyl-, (3aS,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:875240 CAPLUS
DOCUMENT NUMBER: 139:364944
TITLE: Preparation of diketohydrazine derivatives as cysteine protease inhibitors
INVENTOR(S): Hatayama, Akira; Tsuruta, Hiroshi; Ochi, Yasuo; Imawaka, Haruo
PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 231 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003091202	A1	20031106	WO 2003-JP5252		20030424
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2483998	AA	20031106	CA 2003-2483998		20030424
EP 1498411	A1	20050119	EP 2003-723188		20030424
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
BR 2003009670	A	20050315	BR 2003-9670		20030424
PRIORITY APPLN. INFO.:			JP 2002-123796	A	20020425
			WO 2003-JP5252	W	20030424

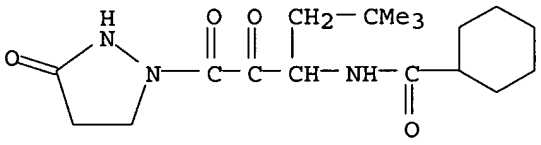
OTHER SOURCE(S): MARPAT 139:364944

AB Diketohydrazine (3-amino-2-oxopropanoylhydrazine or 3-aminopropionohydrazide) derivs. represented by the following general formula R-AA1-AA2-NR9CR7R8COCONR10NRYRX [wherein R = H, CycA, halo, (un)substituted C1-8 alkyl, R16CO, R16C(S), R16O2C, R16R17NCO, R16SO2, R16COCH2, R16C(S)CH2; CycA = C3-15 mono-, bi-, or tricyclic carbocyclic ring, 3- to 15-membered mono-, bi-, or tricyclic heterocyclic ring containing 1-4 N, 1 or 2 O and/or 1 or 2 S atom(s); R16 = each (un)substituted C1-8 alkyl, C2-8 alkenyl, or C2-8 alkynyl, CycA; R17, R9 = H, C1-4 alkyl, CycA,

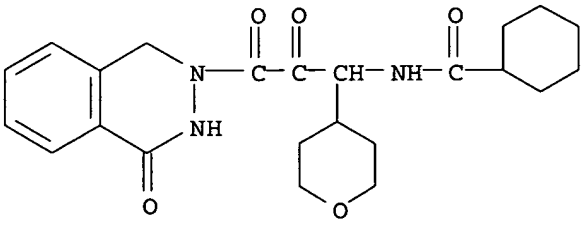
CycA-C1-4 alkyl; AA1 = a single bond, (un)substituted NR3CR1R2CO, etc.; R1, R2 = H, (un)substituted C1-8 alkyl, CysA, etc.; R3, R7, R8 = H, C1-8 alkyl, CycA, CycA-C1-8 alkyl, etc.; AA2 = a single bond, NR3CR1R2CO, -CycC-CO-, -NR38-CycD-CO-, etc.; CycC = 3- to 17-membered mono or bicyclic heterocyclic ring; CycD = C3-14 mono or bicyclic carbocyclic ring, 3- to 14-membered mono- or bicyclic heterocyclic ring; R38 = group listed in R17; R10, RY, and RX are not defined] and pharmaceutically acceptable salts thereof are prepared These compds. are inhibitors of cysteine protease, in particular cathepsin K, S, L, B, H, F, Y, or C, calpain, or caspase 1. Because of having a cysteine protease inhibitory activity, they are useful as remedies for inflammatory diseases, immune diseases, ischemic diseases, respiratory diseases, circulatory diseases, blood diseases, nerve diseases, liver/biliary duct diseases, bone/joint diseases, metabolic diseases, or diseases caused by apoptosis or degradation of bioconstituent proteins. The bone/joint diseases include osteoporosis, chronic articular rheumatism, arthritis, osteoarthritis (arthrosis deformans), hypercalcemia, bone metastasis of carcinoma, or bone fracture. Also disclosed is a bone absorption inhibitor containing the above compound Because of having an elastase inhibitory activity, these compds. are also useful as remedies for COPD (chronic obstructive pulmonary disease) and so on. N'-(3-tert-butyl-1,3-thiazolidin-2-ylidene)-3-cyclohexylcarbonylamino-2-oxo-3-(tetrahydropyran-4-yl)propionohydrazide hydrochloride inhibited cathepsin K with Ki of 2.5 nM. A tablet and an ampule containing N'-(3-methyl-1,3-thiazolidin-2-ylidene)-(3S)-3-cyclohexylcarbonylamino-2-oxo-5-methylhexanohydrazide hydrochloride were described.

IT **620612-47-7P 620612-50-2P 620613-03-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diketohydrazine derivs. as cysteine protease inhibitors and therapeutic agents)

RN 620612-47-7 CAPLUS
CN Cyclohexanecarboxamide, N-[3,3-dimethyl-1-[oxo(3-oxo-1-pyrazolidinyl)acetyl]butyl]- (9CI) (CA INDEX NAME)

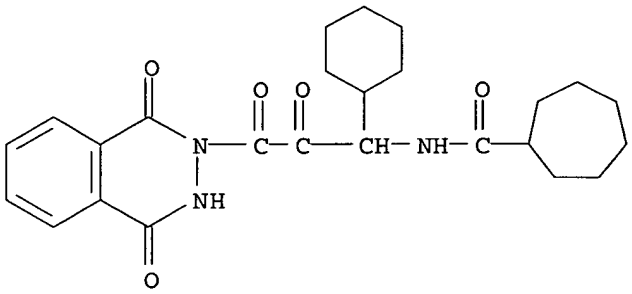


RN 620612-50-2 CAPLUS
CN Cyclohexanecarboxamide, N-[3-(3,4-dihydro-4-oxo-2(1H)-phthalazinyl)-2,3-dioxo-1-(tetrahydro-2H-pyran-4-yl)propyl]- (9CI) (CA INDEX NAME)



RN 620613-03-8 CAPLUS

CN Cycloheptanecarboxamide, N-[1-cyclohexyl-3-(3,4-dihydro-1,4-dioxo-2(1H)-phthalazinyl)-2,3-dioxopropyl]- (9CI) (CA INDEX NAME)

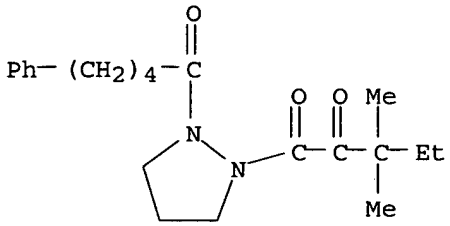


REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

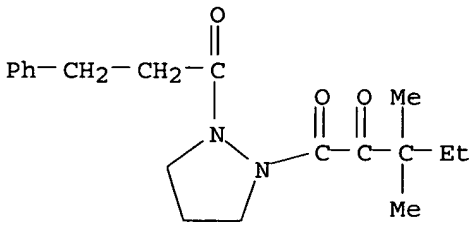
L11 ANSWER 5 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:788599 CAPLUS
DOCUMENT NUMBER: 140:122088
TITLE: Synthesis, molecular modeling and biological evaluation of aza-proline and aza-pipecolic derivatives as FKBP12 ligands and their in vivo neuroprotective effects
AUTHOR(S): Wilkinson, Douglas E.; Thomas, Bert E.; Limburg, David C.; Holmes, Agnes; Sauer, Hansjorg; Ross, Douglas T.; Soni, Raj; Chen, Yi; Guo, Hong; Howorth, Pamela; Valentine, Heather; Spicer, Dawn; Fuller, Mike; Steiner, Joseph P.; Hamilton, Gregory S.; Wu, Yong-Qian
CORPORATE SOURCE: Department of Research, Guilford Pharmaceuticals, Inc., Baltimore, MD, 21224, USA
SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(22), 4815-4825
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:122088
AB Nonimmunosuppressant ligands, exemplified by GPI 1046, for the peptidyl-prolyl isomerase FKBP12 have been found to unexpectedly possess powerful neuroprotective and neuroregenerative effects in vitro and in vivo. We have extensively explored the therapeutic utility of FKBP12 ligands based on analogs of proline and pipecolic acid. As part of our ongoing program to explore novel structural classes of FKBP12 ligands, we herein wish to report a new class of FKBP12 ligands containing aza-proline and aza-pipecolic acid analogs. Details of the synthetic studies, together with biol. activity will be presented.
IT **340255-68-7P 340255-88-1P 340255-89-2P 340255-90-5P 340255-91-6P 340255-92-7P 340255-93-8P 340255-94-9P 340255-95-0P 340255-96-1P 340255-99-4P 340256-00-0P 340256-01-1P 340256-02-2P 340256-03-3P 340256-04-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(aza-proline and aza-pipecolic derivs. as FKBP12 ligands with neuroprotective effects)

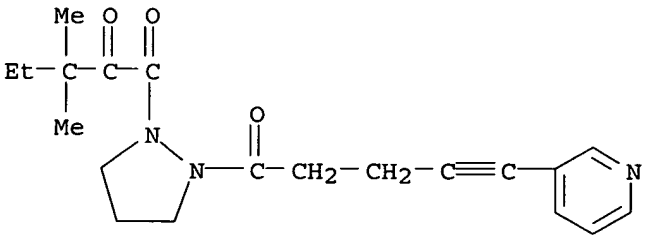
RN 340255-68-7 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-5-phenylpentyl)- (9CI) (CA INDEX NAME)



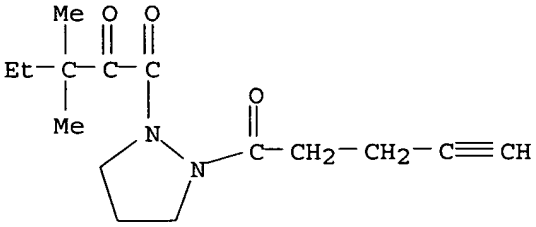
RN 340255-88-1 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-3-phenylpropyl)- (9CI) (CA INDEX NAME)



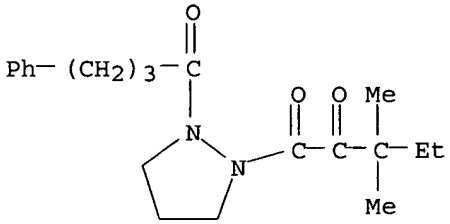
RN 340255-89-2 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-[1-oxo-5-(3-pyridinyl)-4-pentynyl]- (9CI) (CA INDEX NAME)



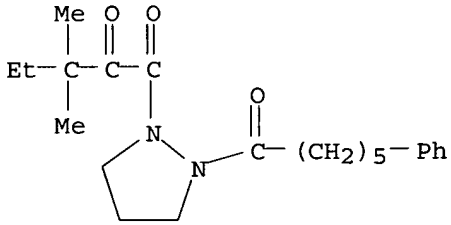
RN 340255-90-5 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-4-pentynyl)- (9CI) (CA INDEX NAME)



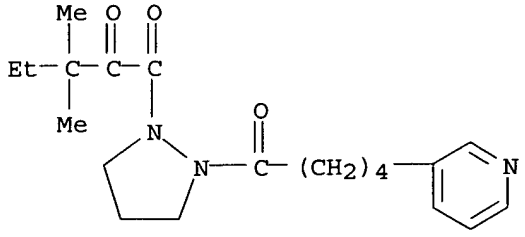
RN 340255-91-6 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-4-phenylbutyl)-(9CI) (CA INDEX NAME)



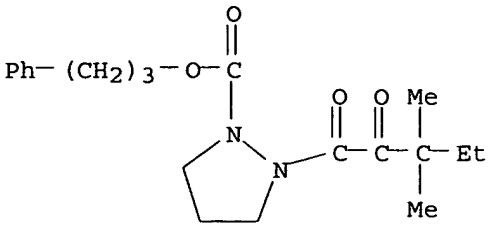
RN 340255-92-7 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-6-phenylhexyl)-(9CI) (CA INDEX NAME)



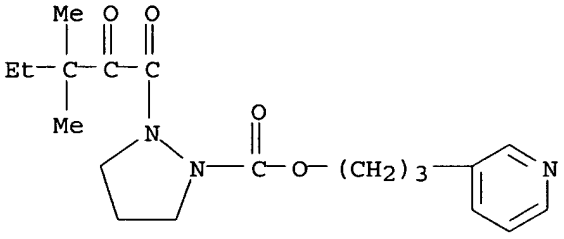
RN 340255-93-8 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-[1-oxo-5-(3-pyridinyl)pentyl]- (9CI) (CA INDEX NAME)



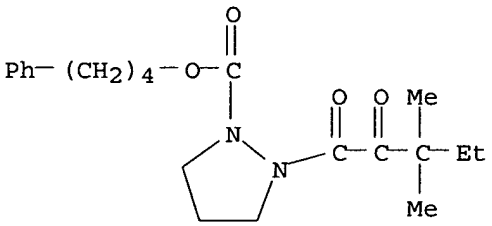
RN 340255-94-9 CAPLUS
CN 1-Pyrazolidinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)-, 3-phenylpropyl ester (9CI) (CA INDEX NAME)



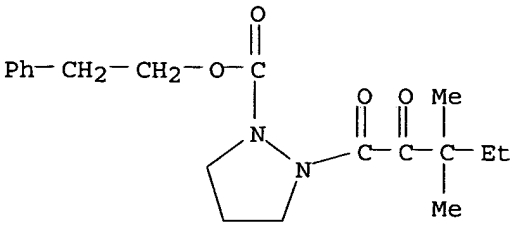
RN 340255-95-0 CAPLUS
CN 1-Pyrazolidinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)-, 3-(3-pyridinyl)propyl ester (9CI) (CA INDEX NAME)



RN 340255-96-1 CAPLUS
CN 1-Pyrazolidinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)-, 4-phenylbutyl ester (9CI) (CA INDEX NAME)

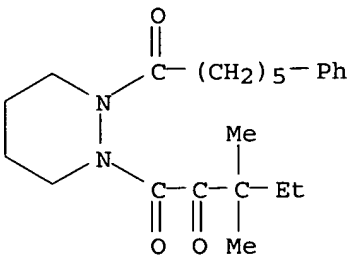


RN 340255-99-4 CAPLUS
CN 1-Pyrazolidinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)-, 2-phenylethyl ester (9CI) (CA INDEX NAME)

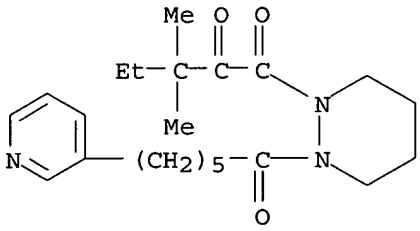


RN 340256-00-0 CAPLUS

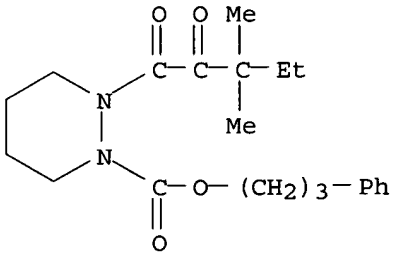
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-(1-oxo-6-phenylhexyl)- (9CI) (CA INDEX NAME)



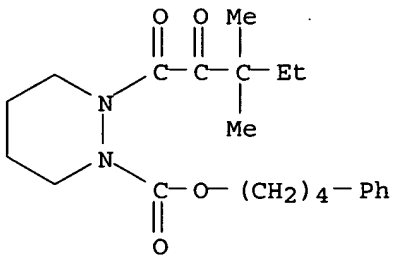
RN 340256-01-1 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-[1-oxo-6-(3-pyridinyl)hexyl]- (9CI) (CA INDEX NAME)



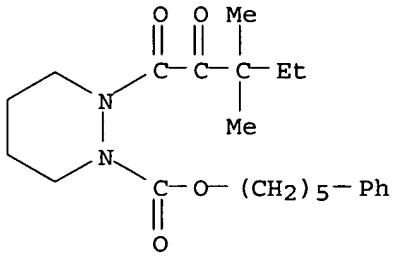
RN 340256-02-2 CAPLUS
CN 1(2H)-Pyridazinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)tetrahydro-, 3-phenylpropyl ester (9CI) (CA INDEX NAME)



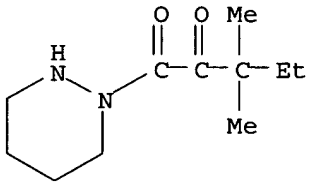
RN 340256-03-3 CAPLUS
CN 1(2H)-Pyridazinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)tetrahydro-, 4-phenylbutyl ester (9CI) (CA INDEX NAME)



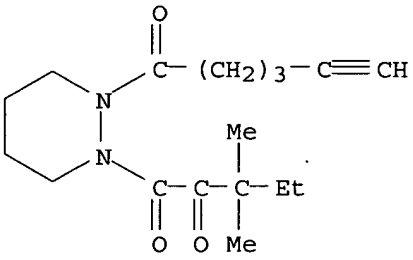
RN 340256-04-4 CAPLUS
CN 1(2H)-Pyridazinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)tetrahydro-, 5-phenylpentyl ester (9CI) (CA INDEX NAME)



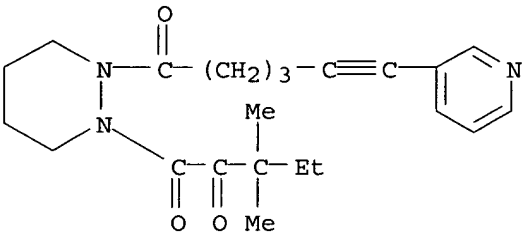
IT **340256-18-0P 340256-19-1P 340256-20-4P**
648958-45-6P 648958-46-7P 648958-47-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(aza-proline and aza-pipecolic derivs. as FKBP12 ligands with neuroprotective effects)
RN 340256-18-0 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro- (9CI) (CA INDEX NAME)



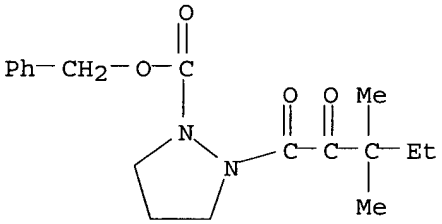
RN 340256-19-1 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-(1-oxo-5-hexynyl)-(9CI) (CA INDEX NAME)



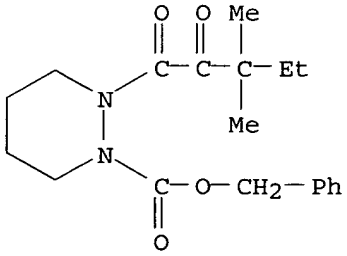
RN 340256-20-4 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-[1-oxo-6-(3-pyridinyl)-5-hexynyl]- (9CI) (CA INDEX NAME)



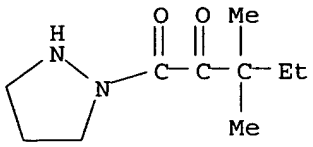
RN 648958-45-6 CAPLUS
CN 1-Pyrazolidinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)



RN 648958-46-7 CAPLUS
CN 1(2H)-Pyridazinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)tetrahydro-, phenylmethyl ester (9CI) (CA INDEX NAME)



RN 648958-47-8 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)- (9CI) (CA INDEX NAME)



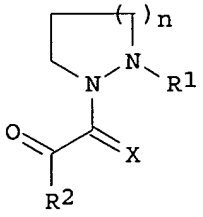
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:172490 CAPLUS
DOCUMENT NUMBER: 136:232310
TITLE: Preparation of N-substituted cyclic aza compounds having neuronal activity
INVENTOR(S): Wu, Yong-qian; Huang, Wei; Hamilton, Gregory S.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 54 pp., Cont.-in-part of U. S. Ser. No. 551,618.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2002028814	A1	20020307	US 2001-835523		20010417
US 6417189	B1	20020709	US 2000-551618		20000417
PRIORITY APPLN. INFO.:			US 1999-164950P	P	19991112
			US 2000-551618	A2	20000417

OTHER SOURCE(S): MARPAT 136:232310
GI

parent



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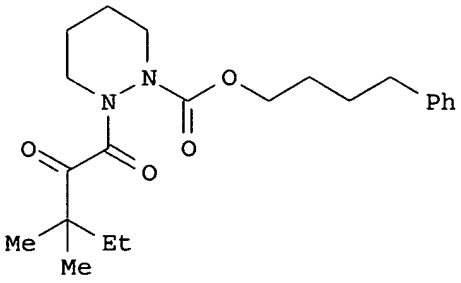
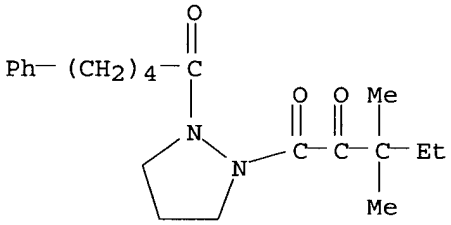


II

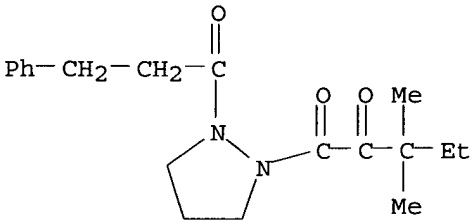
AB Title compds. I [n = 1-3; R1 = CR3, CO2R3, COR3, etc.; R2, R3 = H, alkyl, alkenyl, etc.; X = O, S], useful for effecting neuronal activities, were prepared Thus, II was prepared via a multi-step synthesis from tert-Bu 2-benzylperhydropyridazinecarboxylate. Biol. data for I (results of test for rotamase inhibition and MPTP model of Parkinson's disease) were given. E.g., II possessed a Ki value of 1175 nM in inhibition studies of rotamase and a 14% TH recovery in MPTP models.

IT **340255-68-7P 340255-88-1P 340255-89-2P**
340255-90-5P 340255-91-6P 340255-92-7P
340255-93-8P 340255-94-9P 340255-95-0P
340255-96-1P 340255-99-4P 340256-00-0P
340256-01-1P 340256-02-2P 340256-03-3P
340256-04-4P 340256-07-7P 340256-09-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-substituted cyclic aza compds. having neuronal activity)

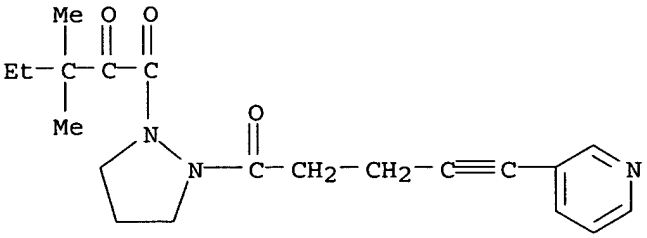
RN 340255-68-7 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-5-phenylpentyl)- (9CI) (CA INDEX NAME)



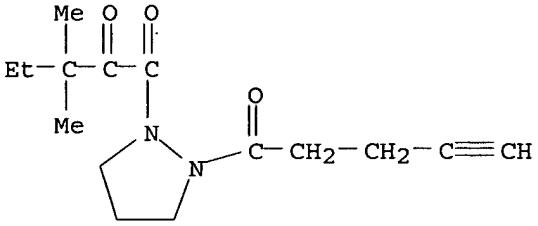
RN 340255-88-1 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-3-phenylpropyl)- (9CI) (CA INDEX NAME)



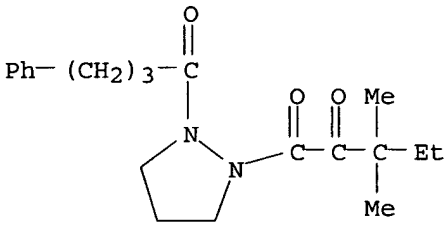
RN 340255-89-2 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-[1-oxo-5-(3-pyridinyl)-4-pentynyl]- (9CI) (CA INDEX NAME)



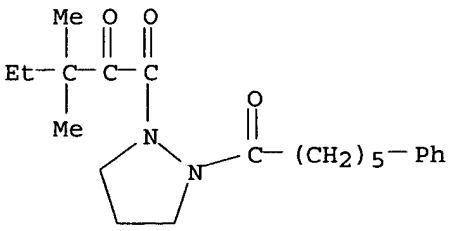
RN 340255-90-5 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-4-pentynyl)- (9CI) (CA INDEX NAME)



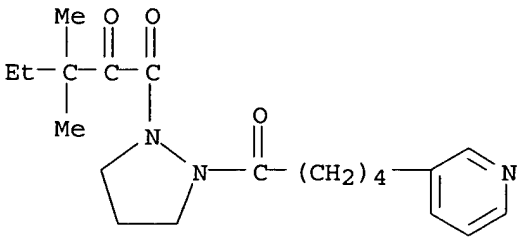
RN 340255-91-6 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-4-phenylbutyl)- (9CI) (CA INDEX NAME)



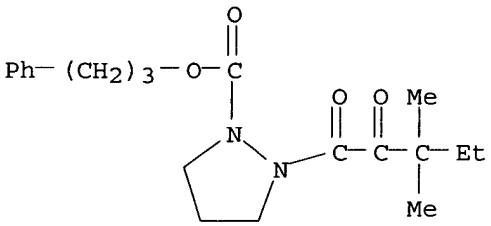
RN 340255-92-7 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-6-phenylhexyl)- (9CI) (CA INDEX NAME)



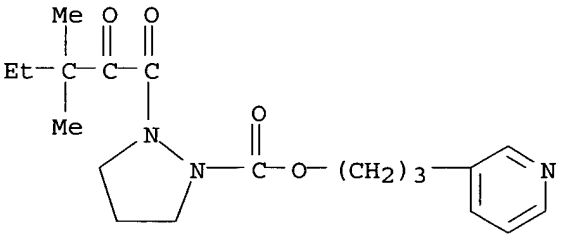
RN 340255-93-8 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-[1-oxo-5-(3-pyridinyl)pentyl]- (9CI) (CA INDEX NAME)



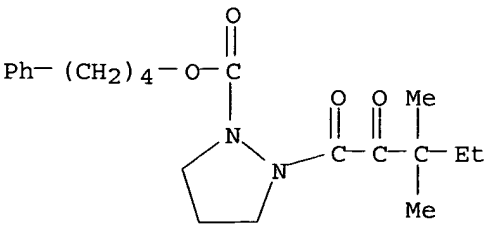
RN 340255-94-9 CAPLUS
CN 1-Pyrazolidinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)-, 3-phenylpropyl ester (9CI) (CA INDEX NAME)



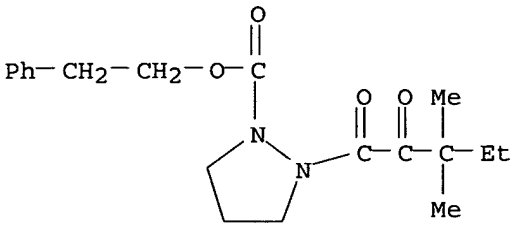
RN 340255-95-0 CAPLUS
CN 1-Pyrazolidinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)-, 3-(3-pyridinyl)propyl ester (9CI) (CA INDEX NAME)



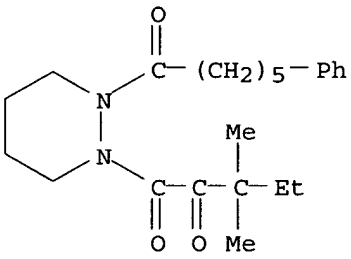
RN 340255-96-1 CAPLUS
CN 1-Pyrazolidinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)-, 4-phenylbutyl ester (9CI) (CA INDEX NAME)



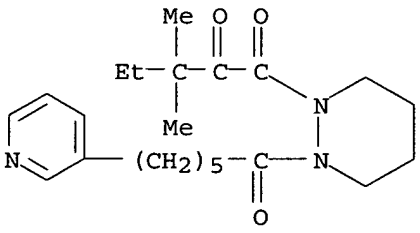
RN 340255-99-4 CAPLUS
CN 1-Pyrazolidinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)-, 2-phenylethyl ester (9CI) (CA INDEX NAME)



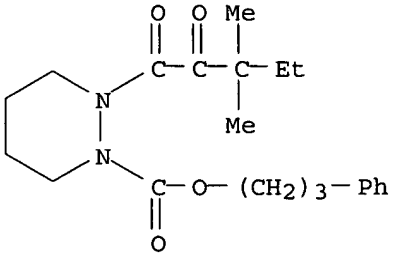
RN 340256-00-0 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-(1-oxo-6-phenylhexyl)- (9CI) (CA INDEX NAME)



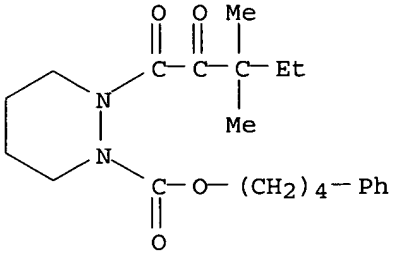
RN 340256-01-1 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-[1-oxo-6-(3-pyridinyl)hexyl]- (9CI) (CA INDEX NAME)



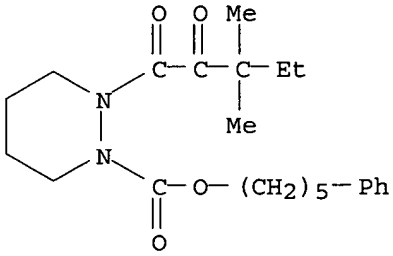
RN 340256-02-2 CAPLUS
CN 1(2H)-Pyridazinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)tetrahydro-, 3-phenylpropyl ester (9CI) (CA INDEX NAME)



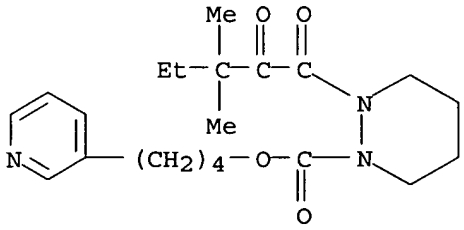
RN 340256-03-3 CAPLUS
CN 1(2H)-Pyridazinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)tetrahydro-, 4-phenylbutyl ester (9CI) (CA INDEX NAME)



RN 340256-04-4 CAPLUS
CN 1(2H)-Pyridazinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)tetrahydro-, 5-phenylpentyl ester (9CI) (CA INDEX NAME)

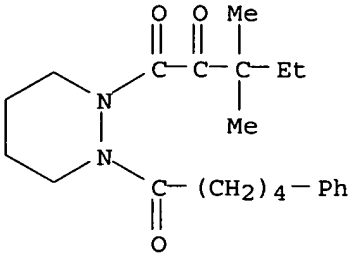


RN 340256-07-7 CAPLUS
CN 1(2H)-Pyridazinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)tetrahydro-, 4-(3-pyridinyl)butyl ester (9CI) (CA INDEX NAME)



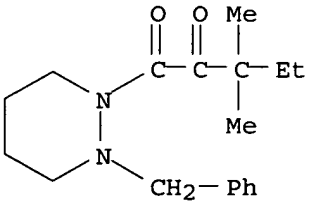
RN 340256-09-9 CAPLUS

CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-(1-oxo-5-phenylpentyl)- (9CI) (CA INDEX NAME)

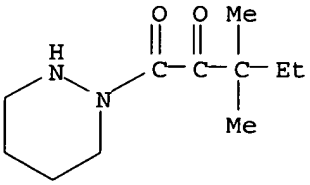


IT **340256-17-9P 340256-18-0P 340256-19-1P 340256-20-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-substituted cyclic aza compds. having neuronal activity)

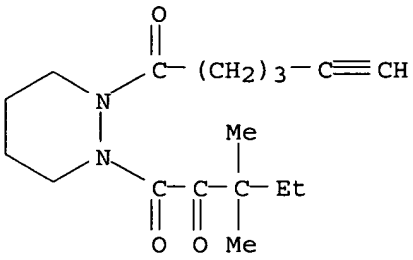
RN 340256-17-9 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-(phenylmethyl)- (9CI) (CA INDEX NAME)



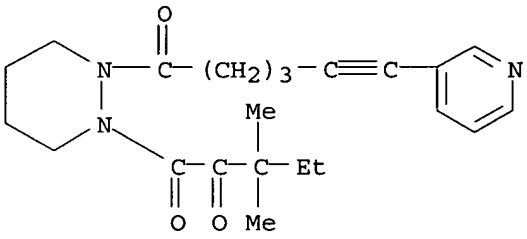
RN 340256-18-0 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro- (9CI) (CA INDEX NAME)



RN 340256-19-1 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-(1-oxo-5-hexynyl)- (9CI) (CA INDEX NAME)



RN 340256-20-4 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-[1-oxo-6-(3-pyridinyl)-5-hexynyl]- (9CI) (CA INDEX NAME)

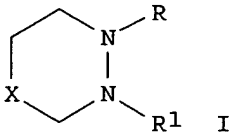


L11 ANSWER 7 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:780859 CAPLUS
DOCUMENT NUMBER: 135:331433
TITLE: Preparation of cyclic diaza compounds for treating neurodegenerative disorders
INVENTOR(S): Wu, Yong-Qian; Huang, Wei; Hamilton, Gregory S.
PATENT ASSIGNEE(S): GPI NIL Holdings, Inc., USA
SOURCE: PCT Int. Appl., 162 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001079177	A1	20011025	WO 2001-US12322	20010417
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6417189	B1	20020709	US 2000-551618	20000417
PRIORITY APPLN. INFO.:			US 2000-551618 A	20000417
			US 1999-164950P P	19991112

OTHER SOURCE(S): MARPAT 135:331433
GI

parent



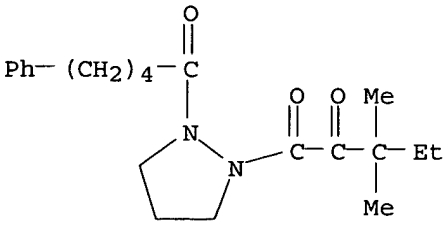
I

AB Title compds. [I;X = bond, CH2; R = COY(CH2)nC6H5, 5-(3-pyridyl)-pent-4-ynoyl, NCCCCH2CH2CO, 5-(3-pyridyl)-pentanoyl, 3-(3-pyridyl)-propoxycarbonyl; Y = O, bond; n = 5, 4, 3, 2; R1 = C6H5CH2SO2, (CH3CH2)(CH3)2CCOCO, C6H5CH2SO2, cyclohexylaminocarbonyl] are prepared for pharmaceutical compns. comprising such compds. and methods of their use for effecting neuronal activities. Thus, the title compound I (X = bond; Y = bond; n = 4; R = COY(CH2)nC6H5; R1 = (CH3CH2)(CH3)2CCOCO) was prepared and biol. tested in mice for MPTP model of Parkinson's disease and showed recovery of TH-stained dopaminergic neurons.

IT **340255-68-7P 340255-88-1P 340255-89-2P**
340255-91-6P 340255-92-7P 340255-93-8P
340255-94-9P 340255-95-0P 340255-96-1P
340255-99-4P 340256-00-0P 340256-01-1P
340256-02-2P 340256-03-3P 340256-04-4P
340256-07-7P 340256-09-9P 369390-81-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclic diaza compds. for treating neurodegenerative disorders)

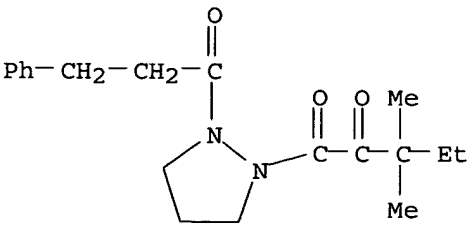
RN 340255-68-7 CAPLUS

CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-5-phenylpentyl)- (9CI) (CA INDEX NAME)

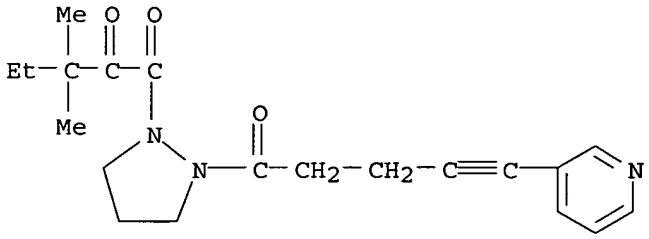


RN 340255-88-1 CAPLUS

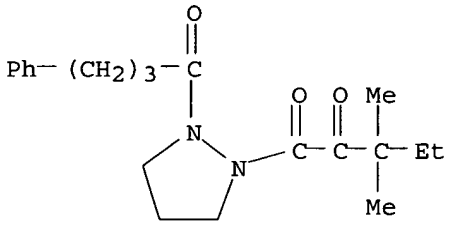
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-3-phenylpropyl)- (9CI) (CA INDEX NAME)



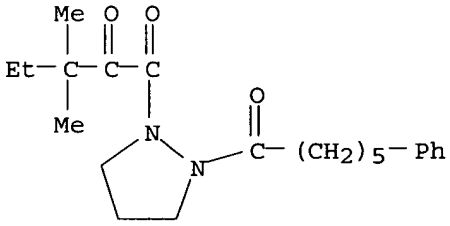
RN 340255-89-2 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-[1-oxo-5-(3-pyridinyl)-4-pentynyl]- (9CI) (CA INDEX NAME)



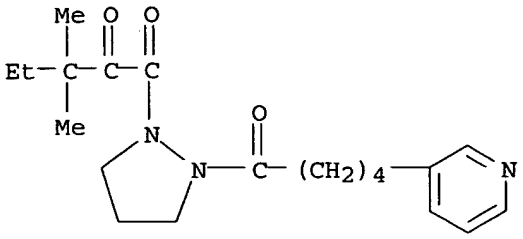
RN 340255-91-6 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-4-phenylbutyl)- (9CI) (CA INDEX NAME)



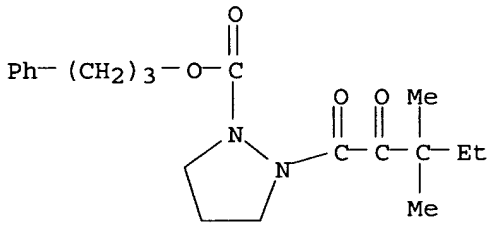
RN 340255-92-7 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-6-phenylhexyl)- (9CI) (CA INDEX NAME)



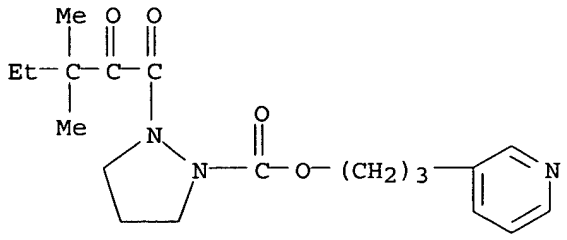
RN 340255-93-8 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-[1-oxo-5-(3-pyridinyl)pentyl]- (9CI) (CA INDEX NAME)



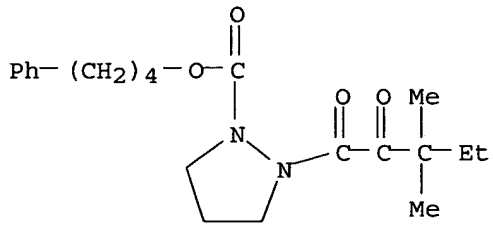
RN 340255-94-9 CAPLUS
CN 1-Pyrazolidinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)-, 3-phenylpropyl ester (9CI) (CA INDEX NAME)



RN 340255-95-0 CAPLUS
CN 1-Pyrazolidinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)-, 3-(3-pyridinyl)propyl ester (9CI) (CA INDEX NAME)

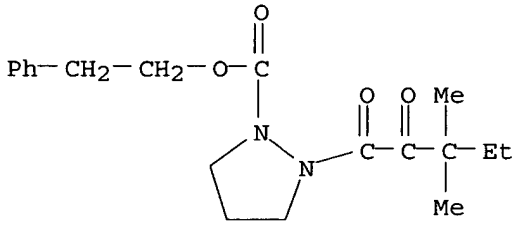


RN 340255-96-1 CAPLUS
CN 1-Pyrazolidinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)-, 4-phenylbutyl ester (9CI) (CA INDEX NAME)

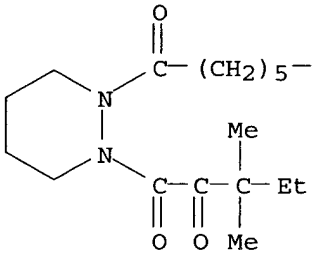


RN 340255-99-4 CAPLUS
CN 1-Pyrazolidinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)-,

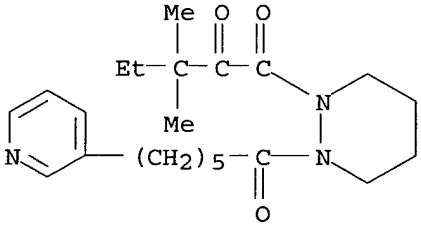
2-phenylethyl ester (9CI) (CA INDEX NAME)



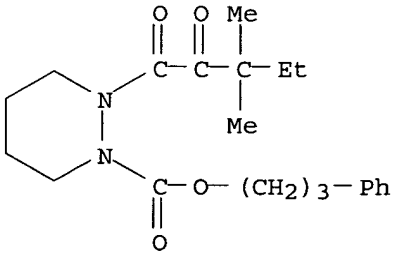
RN 340256-00-0 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-(1-oxo-6-phenylhexyl)- (9CI) (CA INDEX NAME)



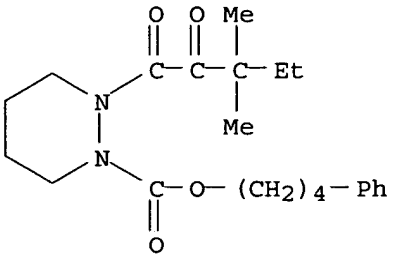
RN 340256-01-1 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-[1-oxo-6-(3-pyridinyl)hexyl]- (9CI) (CA INDEX NAME)



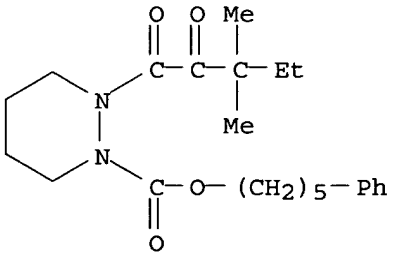
RN 340256-02-2 CAPLUS
CN 1(2H)-Pyridazinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)tetrahydro-, 3-phenylpropyl ester (9CI) (CA INDEX NAME)



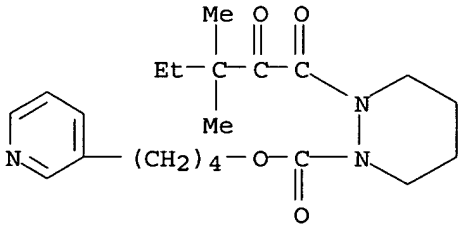
RN 340256-03-3 CAPLUS
CN 1(2H)-Pyridazinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)tetrahydro-, 4-phenylbutyl ester (9CI) (CA INDEX NAME)



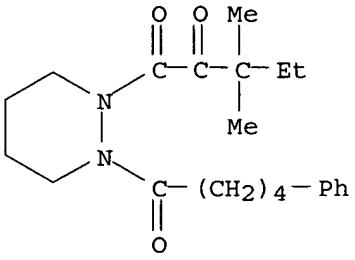
RN 340256-04-4 CAPLUS
CN 1(2H)-Pyridazinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)tetrahydro-, 5-phenylpentyl ester (9CI) (CA INDEX NAME)



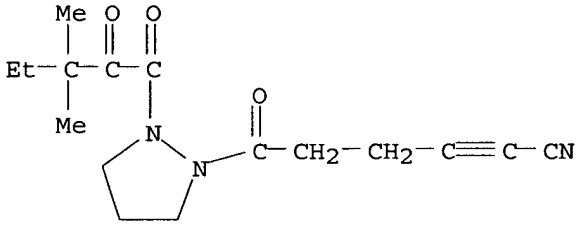
RN 340256-07-7 CAPLUS
CN 1(2H)-Pyridazinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)tetrahydro-, 4-(3-pyridinyl)butyl ester (9CI) (CA INDEX NAME)



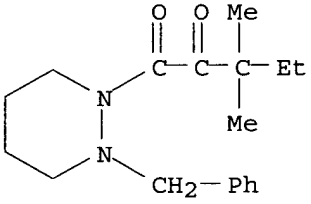
RN 340256-09-9 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-(1-oxo-5-phenylpentyl)- (9CI) (CA INDEX NAME)



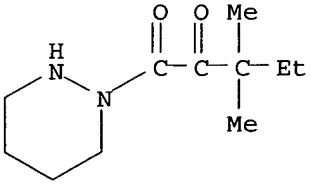
RN 369390-81-8 CAPLUS
CN Pyrazolidine, 1-(5-cyano-1-oxo-4-pentynyl)-2-(3,3-dimethyl-1,2-dioxopentyl)- (9CI) (CA INDEX NAME)



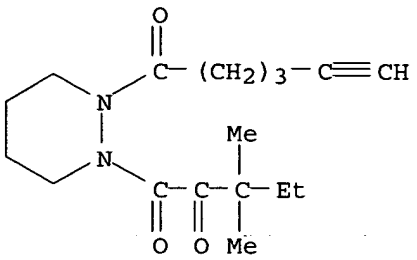
IT **340256-17-9P 340256-18-0P 340256-19-1P 340256-20-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclic diaza compds. for treating neurodegenerative disorders)
RN 340256-17-9 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-(phenylmethyl)- (9CI) (CA INDEX NAME)



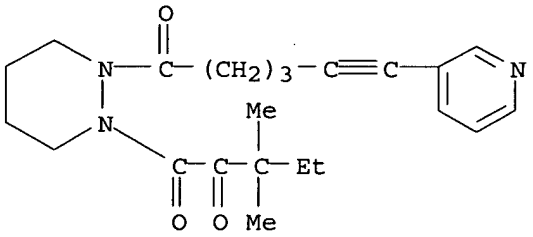
RN 340256-18-0 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro- (9CI) (CA INDEX NAME)



RN 340256-19-1 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-(1-oxo-5-hexynyl)-(9CI) (CA INDEX NAME)



RN 340256-20-4 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-[1-oxo-6-(3-pyridinyl)-5-hexynyl]- (9CI) (CA INDEX NAME)



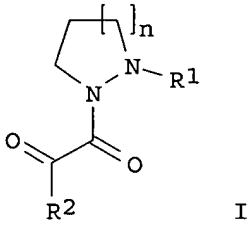
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 8 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:380557 CAPLUS
DOCUMENT NUMBER: 134:366884
TITLE: Preparation of N-substituted cyclic aza compounds having neuronal activity
INVENTOR(S): Wu, Yong-Qian; Huang, Wei; Hamilton, Gregory S.
PATENT ASSIGNEE(S): GPI Nil Holdings, Inc., USA
SOURCE: PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001036388	A1	20010525	WO 2000-US23603	20000828
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,				

	CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6417189	B1	20020709	US 2000-551618	20000417
	CA 2390071	AA	20010525	CA 2000-2390071	20000828
	EP 1242383	A1	20020925	EP 2000-957870	20000828
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	JP 2003514799	T2	20030422	JP 2001-538878	20000828
	AU 781740	B2	20050609	AU 2000-69428	20000828
PRIORITY APPLN. INFO.:				US 1999-164950P	P 19991112
				US 2000-551618	A 20000417
				WO 2000-US23603	W 20000828

OTHER SOURCE(S): MARPAT 134:366884
GI



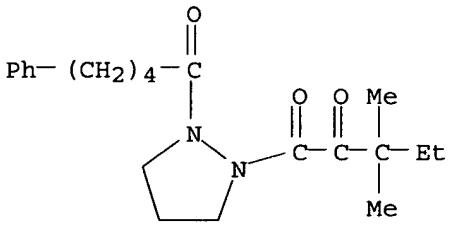
I

AB The title compds. [I; n = 1-3; R1 = CR3, CO2R3, COR3, etc.; R2, R3 = H, alkyl, alkenyl, etc.; X = O, S], useful for effecting neuronal activities, were prepared E.g., a multi-step synthesis of I [n = 2; R1 = CO2(CH2)4Ph; R2 = CMe2Et; X = O] was described. Biol. data for compds. I (results of test for rotamase inhibition and MPTP model of Parkinson's disease) were given.

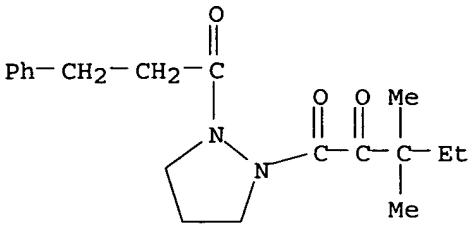
IT **340255-68-7P 340255-88-1P 340255-89-2P**
340255-90-5P 340255-91-6P 340255-92-7P
340255-93-8P 340255-94-9P 340255-95-0P
340255-96-1P 340255-99-4P 340256-00-0P
340256-01-1P 340256-02-2P 340256-03-3P
340256-04-4P 340256-07-7P 340256-09-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-substituted cyclic aza compds. having neuronal activity)

RN 340255-68-7 CAPLUS

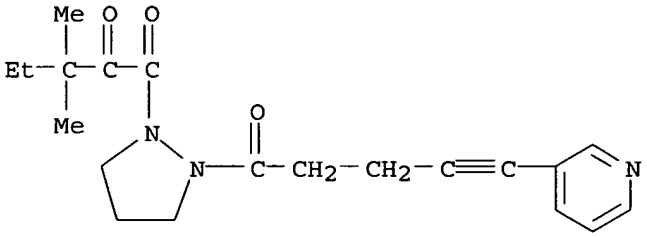
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-5-phenylpentyl)- (9CI) (CA INDEX NAME)



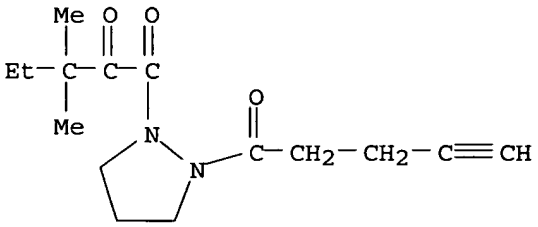
RN 340255-88-1 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-3-phenylpropyl)- (9CI) (CA INDEX NAME)



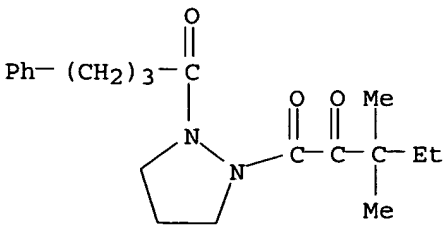
RN 340255-89-2 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-[1-oxo-5-(3-pyridinyl)-4-pentynyl]- (9CI) (CA INDEX NAME)



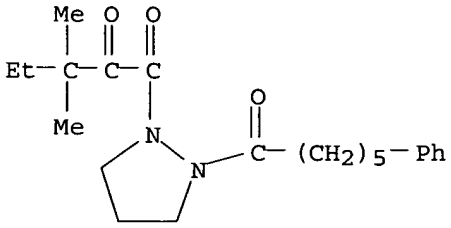
RN 340255-90-5 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-4-pentynyl)- (9CI) (CA INDEX NAME)



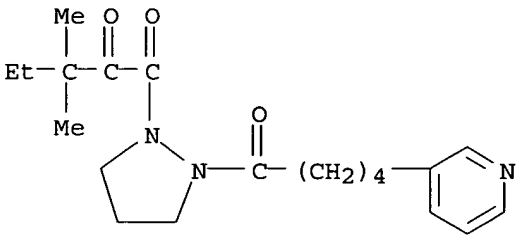
RN 340255-91-6 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-4-phenylbutyl)- (9CI) (CA INDEX NAME)



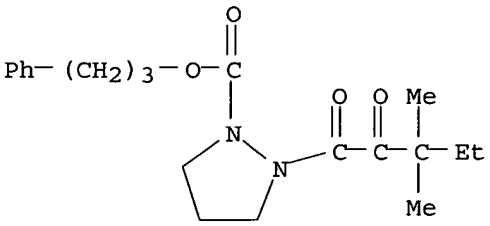
RN 340255-92-7 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-(1-oxo-6-phenylhexyl)-(9CI) (CA INDEX NAME)



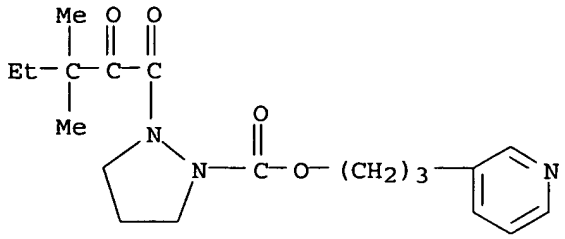
RN 340255-93-8 CAPLUS
CN Pyrazolidine, 1-(3,3-dimethyl-1,2-dioxopentyl)-2-[1-oxo-5-(3-pyridinyl)pentyl]- (9CI) (CA INDEX NAME)



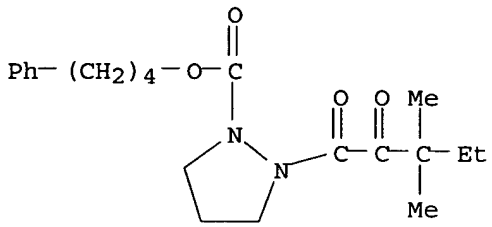
RN 340255-94-9 CAPLUS
CN 1-Pyrazolidinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)-, 3-phenylpropyl ester (9CI) (CA INDEX NAME)



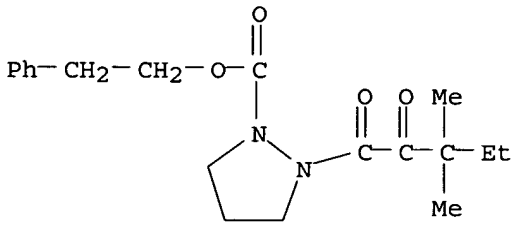
RN 340255-95-0 CAPLUS
CN 1-Pyrazolidinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)-, 3-(3-pyridinyl)propyl ester (9CI) (CA INDEX NAME)



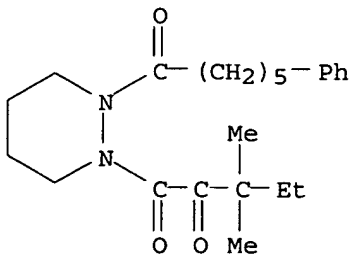
RN 340255-96-1 CAPLUS
CN 1-Pyrazolidinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)-, 4-phenylbutyl ester (9CI) (CA INDEX NAME)



RN 340255-99-4 CAPLUS
CN 1-Pyrazolidinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)-, 2-phenylethyl ester (9CI) (CA INDEX NAME)

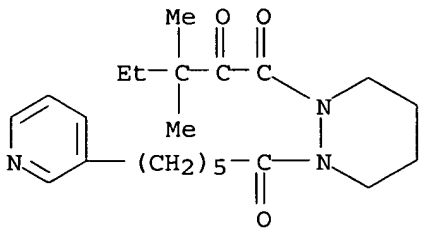


RN 340256-00-0 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-(1-oxo-6-phenylhexyl)- (9CI) (CA INDEX NAME)

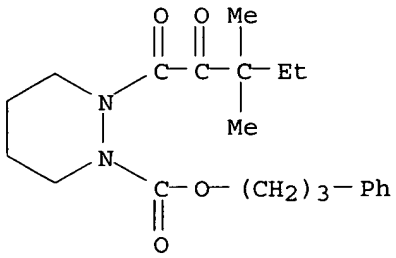


RN 340256-01-1 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-[1-oxo-6-(3-

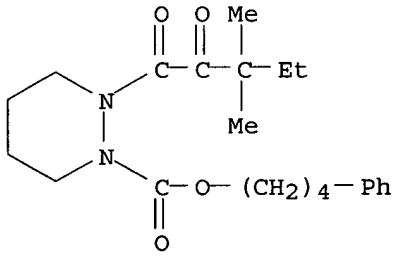
pyridinyl)hexyl]- (9CI) (CA INDEX NAME)



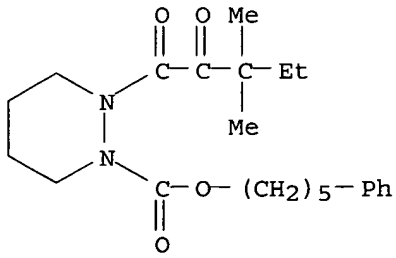
RN 340256-02-2 CAPLUS
CN 1(2H)-Pyridazinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)tetrahydro-, 3-phenylpropyl ester (9CI) (CA INDEX NAME)



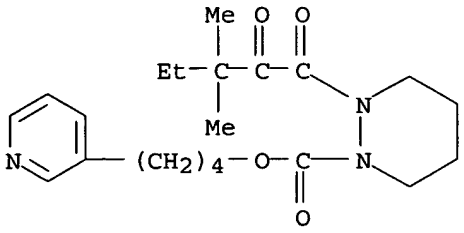
RN 340256-03-3 CAPLUS
CN 1(2H)-Pyridazinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)tetrahydro-, 4-phenylbutyl ester (9CI) (CA INDEX NAME)



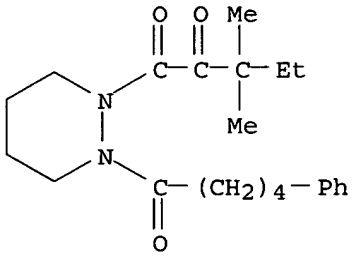
RN 340256-04-4 CAPLUS
CN 1(2H)-Pyridazinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)tetrahydro-, 5-phenylpentyl ester (9CI) (CA INDEX NAME)



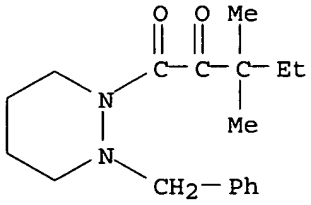
RN 340256-07-7 CAPLUS
CN 1(2H)-Pyridazinecarboxylic acid, 2-(3,3-dimethyl-1,2-dioxopentyl)tetrahydro-, 4-(3-pyridinyl)butyl ester (9CI) (CA INDEX NAME)



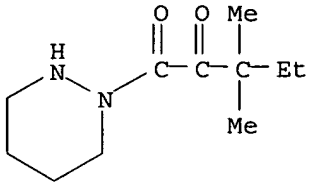
RN 340256-09-9 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-(1-oxo-5-phenylpentyl)- (9CI) (CA INDEX NAME)



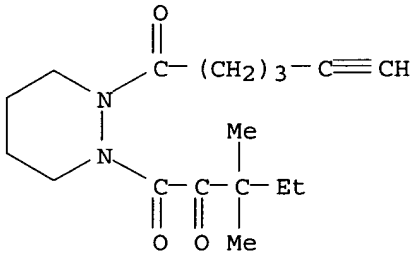
IT **340256-17-9P 340256-18-0P 340256-19-1P**
340256-20-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-substituted cyclic aza compds. having neuronal activity)
RN 340256-17-9 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-(phenylmethyl)- (9CI) (CA INDEX NAME)



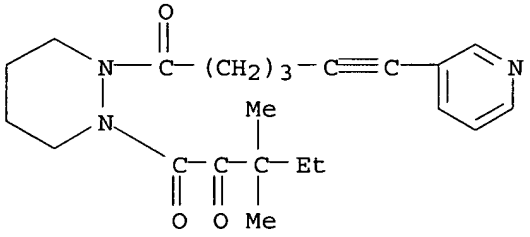
RN 340256-18-0 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro- (9CI) (CA INDEX NAME)



RN 340256-19-1 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-(1-oxo-5-hexynyl)-(9CI) (CA INDEX NAME)



RN 340256-20-4 CAPLUS
CN Pyridazine, 1-(3,3-dimethyl-1,2-dioxopentyl)hexahydro-2-[1-oxo-6-(3-pyridinyl)-5-hexynyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

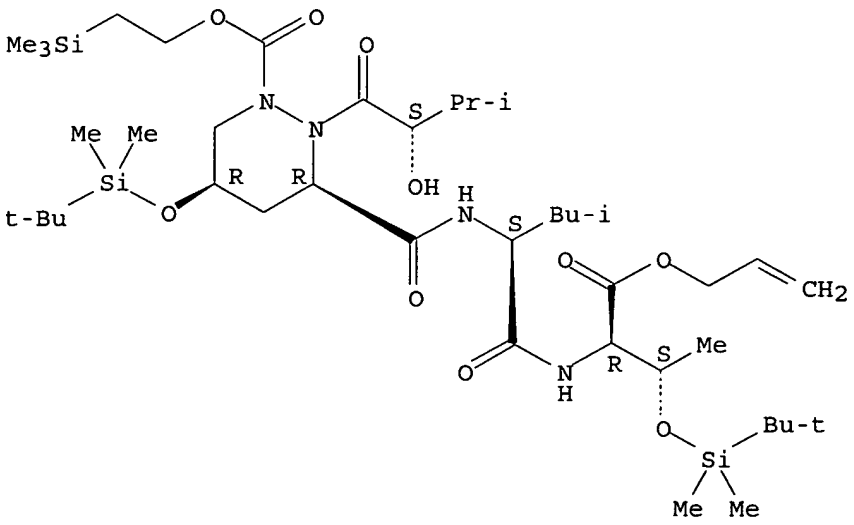
L11 ANSWER 9 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:57793 CAPLUS
DOCUMENT NUMBER: 134:237812
TITLE: Discovery through total synthesis: a retrospective on the himastatin problem
AUTHOR(S): Kamenecka, Theodore M.; Danishefsky, Samuel J.
CORPORATE SOURCE: Laboratory for Bioorganic Chemistry, Sloan-Kettering Institute for Cancer Research, New York, NY, 10021, USA
SOURCE: Chemistry--A European Journal (2001), 7(1), 41-63
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:237812
AB A total synthesis of a structure proposed for himastatin was accomplished.

The non-identity of the fully synthetic material with himastatin necessitated a revision of the assigned structure. Confirmation of the revised stereostructure was subsequently confirmed through total synthesis. Among the achievements during this effort were i: stereospecific routes to both anti-cis and syn-cis pyrrolindoline substructures; ii: a practical synthesis to 5-hydroxypiperazic acid in enantiomerically pure form; iii: a Stille coupling leading to a complex bi-indole moiety, and iv: efficient protecting group management throughout the evolving depsipeptide domain. The outlines for a biol. pharmacophore have been delineated. The alternating D- and L-substituents in the 6-mer as well as the biaryl linkage connecting the two identical subunits are critical for maintaining biol. activity. This pattern is simulated in another antibiotic, and suggests a possible structural trend for future SAR investigations.

IT **329786-81-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and stereo determination of himastatin by total synthesis methods)

RN 329786-81-4 CAPLUS
CN D-Threonine, (2S)-2-hydroxy-3-methylbutanoyl-(3R,5R)-5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexahydro-1-[[2-(trimethylsilyl)ethoxy]carbonyl]-3-pyridazinecarbonyl-L-leucyl-O-[(1,1-dimethylethyl)dimethylsilyl]-, 2-propenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 10 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:794787 CAPLUS
DOCUMENT NUMBER: 130:110633
TITLE: Total synthesis of himastatin: confirmation of the revised stereostructure
AUTHOR(S): Kamenecka, Theodore M.; Danishefsky, Samuel J.
CORPORATE SOURCE: Laboratory for Bioorganic Chemistry, Sloan-Kettering Institute for Cancer Research, New York, NY, 10021,

USA
SOURCE: Angewandte Chemie, International Edition (1998), 37(21), 2995-2998
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

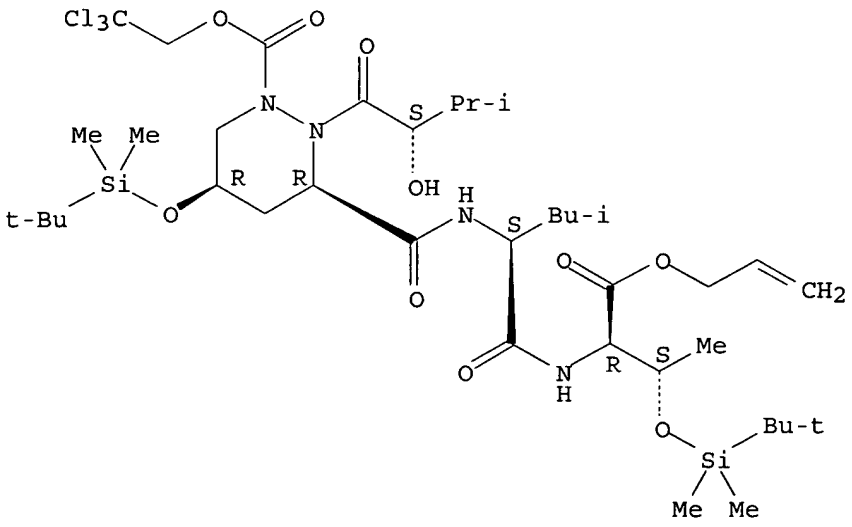
AB A total synthesis of the cyclodepsipeptide himastatin (I) is described, confirming the revised stereostructure. A cyclodepsipeptide corresponding to the monomeric parent pyrroloindoline system was also prepared

IT **219646-81-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis of himastatin and confirmation of revised stereostructure)

RN 219646-81-8 CAPLUS

CN D-Threonine, (2S)-2-hydroxy-3-methylbutanoyl-(3R,5R)-5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexahydro-1-[(2,2,2-trichloroethoxy)carbonyl]-3-pyridazinecarbonyl-L-leucyl-O-[(1,1-dimethylethyl)dimethylsilyl]-, 2-propenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 11 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:619195 CAPLUS
DOCUMENT NUMBER: 127:339205
TITLE: Silver halide photographic material containing precursor for photographically useful compound

INVENTOR(S): Kawagishi, Toshio; Tsukahara, Jiro; Sato, Hideaki; Uchida, Osamu; Nakai, Yasushi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 49 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

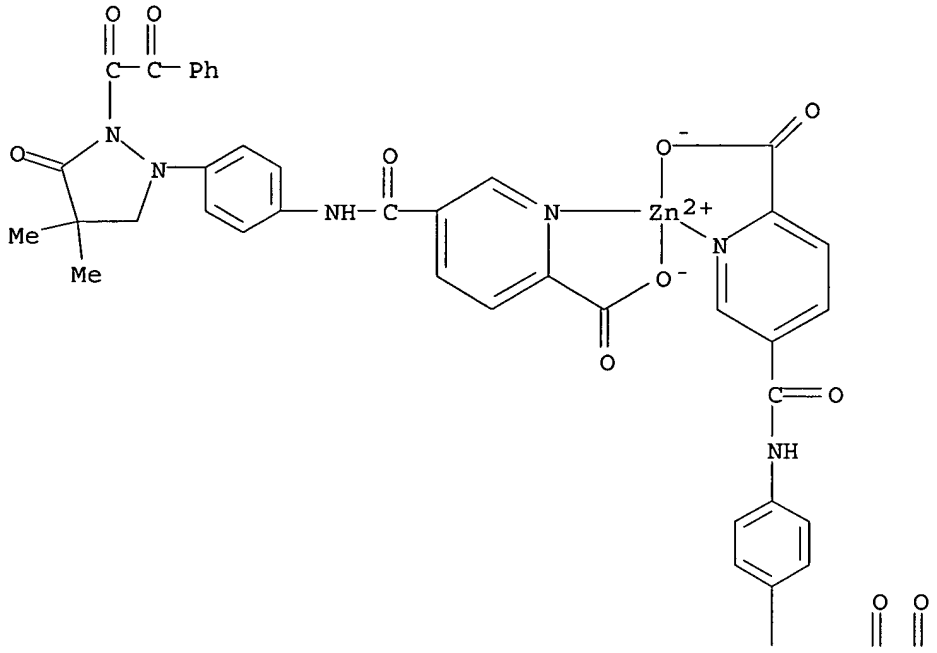
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09244192	A2	19970919	JP 1996-53315	19960311
PRIORITY APPLN. INFO.:			JP 1996-53315	19960311

AB Claimed Ag halide photog. material contains a precursor for photog. useful compound (PUG) (BP-L-LIG)k-M, where BP is the residue of the PUG, L is a bivalent linkage or chemical bond; LIG is multidentated ligand residue; k is an integer of 1-3; and M is selected from Li, B, Mg, Ca, Sc, Ti, Fe, Ni, Cu and Zn. Preferable Ms are Zn and Cu, and preferable BPs are 1-phenyl-3-pyrazolidones blocked at 2- or 3-site. Other PUG includes development inhibitor such as imidazoles, triazoles and tetrazoles, and development accelerator such as hydrazine derivs. The precursor has adequate preprocessing storage stability, while with rapid release of BP at the development stage. The precursor is suitable incorporated in multilayer color neg. films. Thus, Zn chelate of bis[1-[p-(3-carboxy-4-hydroxy-benzoylamino)phenyl]-2-(2-aceto-2,2-dimethyl-aceto)-4,4-dimethyl-3-pyrazolidone] was incorporated in a multilayer color neg. film to provide the mentioned advantages.

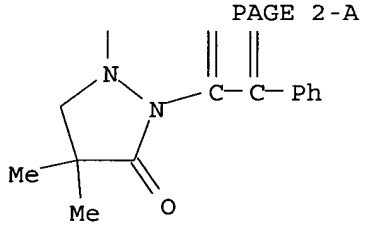
IT **197863-41-5P**
RL: DEV (Device component use); PNU (Preparation, unclassified); PREP (Preparation); USES (Uses)
(photog. material containing precursor for photog. useful compound having good storage stability)

RN 197863-41-5 CAPLUS
CN Zinc, bis[5-[[[4-[4,4-dimethyl-3-oxo-2-(oxophenylacetyl)-1-pyrazolidinyl]phenyl]amino]carbonyl]-2-pyridinecarboxylato-κN1,κO2]-, (T-4)- (9CI) (CA INDEX NAME)

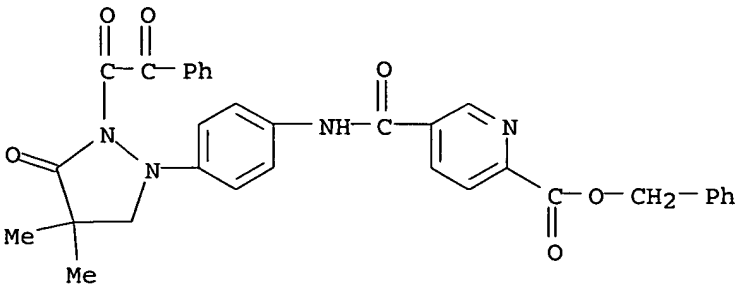
PAGE 1-A



PAGE 2-A



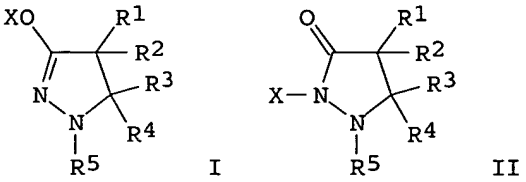
IT **197863-48-2P**
RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of; precursor for photog. useful compound from)
RN 197863-48-2 CAPLUS
CN 2-Pyridinecarboxylic acid, 5-[[[4-[4,4-dimethyl-3-oxo-2-(oxophenylacetyl)-1-pyrazolidinyl]phenyl]amino]carbonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



L11 ANSWER 12 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:570816 CAPLUS
DOCUMENT NUMBER: 115:170816
TITLE: Heat-developable light-sensitive material
INVENTOR(S): Taguchi, Toshiki; Nakamine, Takeshi; Ito, Takayuji; Nakamura, Koki; Mikoshiba, Hisashi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 99 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 418743	A2	19910327	EP 1990-117690	19900913
EP 418743	A3	19910515		
R: DE, FR, GB, IT, NL				
JP 03102345	A2	19910426	JP 1989-240963	19890918
JP 03131848	A2	19910605	JP 1989-269556	19891017
JP 2612206	B2	19970521		
JP 03160443	A2	19910710	JP 1989-301076	19891120
JP 2612207	B2	19970521		

PRIORITY APPLN. INFO.: JP 1989-240963 A 19890918
JP 1989-269556 A 19891017
JP 1989-301076 A 19891120
OTHER SOURCE(S): MARPAT 115:170816
GI

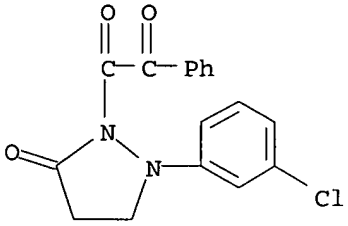


I II

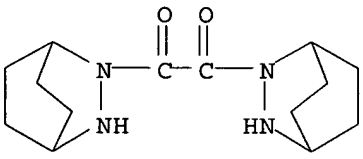
AB The title material comprises photosensitive Ag halide, a binder, and a reducing agent having a m.p. ≤120° and a mol. formula I or II [R1-R4 = H, alkyl, aryl, heterocyclic group; R5 = aryl, heterocyclic group; x = alkyl acyl, alkoxycarbonyl, aryloxycarbonyl, carbamoyl, sulfamoyl, diketone, hydrobenzofuranone derivative]. A color photog. material

for heat development comprises a dye precursor and an electron donor from a glyoxylic acid Ph ester derivative or a carboxylic acid Ph ester derivative The material has excellent shelf life and is capable of obtaining images having good discrimination.

IT **136468-25-2**
RL: USES (Uses)
(reducing agent, heat-developable photog. material containing)
RN 136468-25-2 CAPLUS
CN 3-Pyrazolidinone, 1-(3-chlorophenyl)-2-(oxophenylacetyl)- (9CI) (CA INDEX NAME)

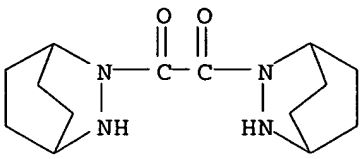


L11 ANSWER 13 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:5637 CAPLUS
DOCUMENT NUMBER: 114:5637
TITLE: The synthesis and study of acylated bishydrazines and their radical cations for their mixed valence behavior and the study of solvent effects on self-electron-transfer rate constants for a sesquibicyclic hydrazine
AUTHOR(S): Kim, Yaesil
CORPORATE SOURCE: Univ. Wisconsin, Madison, WI, USA
SOURCE: (1989) 282 pp. Avail.: Univ. Microfilms Int., Order No. DA9013353
From: Diss. Abstr. Int. B 1990, 51(1), 213
DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable
IT **130973-68-1P**
RL: PREP (Preparation)
(formation, crystallog., and mixed valence behavior of)
RN 130973-68-1 CAPLUS
CN 2,3-Diazabicyclo[2.2.2]octane, 2,2'-(1,2-dioxo-1,2-ethanediyl)bis-, radical ion(1+) (9CI) (CA INDEX NAME)

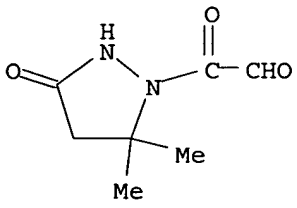


IT **130973-67-0**
RL: PRP (Properties)
(oxidation potential of)

RN 130973-67-0 CAPLUS
CN 2,3-Diazabicyclo[2.2.2]octane, 2,2'-(1,2-dioxo-1,2-ethanediyl)bis- (9CI) (CA INDEX NAME)



L11 ANSWER 14 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1989:593900 CAPLUS
DOCUMENT NUMBER: 111:193900
TITLE: Reactivity of pyrazolones toward hydroxyl radical and O2•-
AUTHOR(S): Pirumyan, G. P.; Martiryan, A. I.; Skurlatov, Yu. I.; Shtamm, E. V.; Nalbandyan, D. M.
CORPORATE SOURCE: Erevan. Gos. Univ., Yerevan, USSR
SOURCE: Armyanskii Khimicheskii Zhurnal (1989), 42(2), 71-6
CODEN: AYKZAN; ISSN: 0515-9628
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Reactivity of pyrazolines of importance to the fishing industry with HO• and O2•- was assessed by their effect on bleaching of the dye p-nitrosodimethylaniline induced by H2O2 photolysis.
IT **123475-95-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of, with hydroxyl radical and superoxide, kinetics of)
RN 123475-95-6 CAPLUS
CN 3-Pyrazolidinone, 5,5-dimethyl-1-(oxoacetyl)- (9CI) (CA INDEX NAME)



L11 ANSWER 15 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1987:119880 CAPLUS
DOCUMENT NUMBER: 106:119880
TITLE: 7-Substituted bicyclic pyrazolidinones, their preparation, and their use as antibacterials
INVENTOR(S): Jungheim, Louis Nickolaus; Sigmund, Sandra Kay; Holmes, Richard Elmer; Barnett, Charles Jackson; Ternansky, Robert John
PATENT ASSIGNEE(S): Eli Lilly and Co., USA
SOURCE: Eur. Pat. Appl., 337 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English

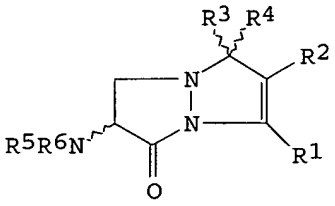
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 202046	A1	19861120	EP 1986-303174	19860428
EP 202046	B1	19910130		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
CN 86103619	A	19861029	CN 1986-103619	19860428
AU 8656755	A1	19861113	AU 1986-56755	19860428
DK 8601930	A	19870120	DK 1986-1930	19860428
HU 40660	A2	19870128	HU 1986-1763	19860428
ZA 8603170	A	19871230	ZA 1986-3170	19860428
ES 554463	A1	19880216	ES 1986-554463	19860428
CA 1274832	A1	19901002	CA 1986-507777	19860428
AT 60605	E	19910215	AT 1986-303174	19860428
JP 61254589	A2	19861112	JP 1986-100817	19860430
JP 07059582	B4	19950628		
US 4716232	A	19871229	US 1986-862913	19860514
US 4734505	A	19880329	US 1986-862909	19860514
US 4734504	A	19880329	US 1986-862918	19860514
JP 63112583	A2	19880517	JP 1986-258084	19861028
US 4795815	A	19890103	US 1987-114897	19871029
ZA 8802604	A	19891227	ZA 1988-2604	19880413
US 4940718	A	19900710	US 1989-418782	19891002
US 5011938	A	19910430	US 1990-503574	19900403

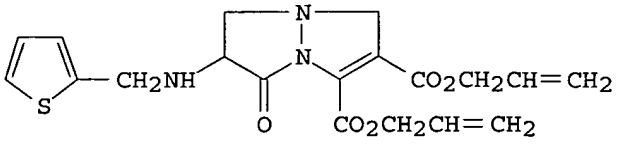
PRIORITY APPLN. INFO.:

US 1985-729021	A	19850430
EP 1986-303174	A	19860428
US 1986-862906	B2	19860514
US 1986-862916	A1	19860514
US 1987-42196	A2	19870423
US 1987-103488	B1	19870930
US 1989-418782	A3	19891002

GI



I



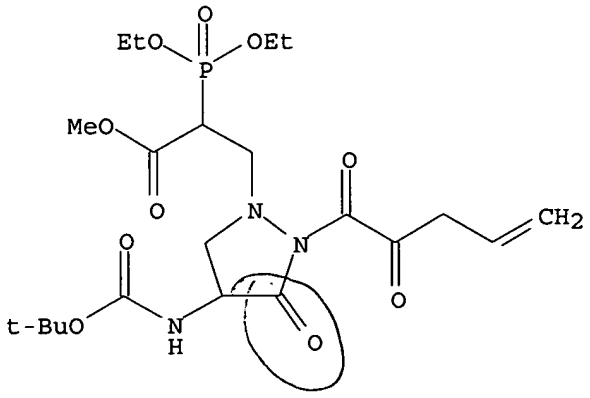
II

AB The title compds. I [1 of R1, R2 = H, halo, C1-6 (un)substituted alkyl, perfluoro C2-4 alkyl, C7-12 (un)substituted aralkyl, (un)substituted Ph, heterocyclyl, NO2, cyano, CX3 (X = F, Cl, Br, iodo), S(O)zR7 [z = 0-2; R7 = C1-6 (un)substituted alkyl, Ph, C7-12 arylalkyl, heterocyclyl], COR8 [R8

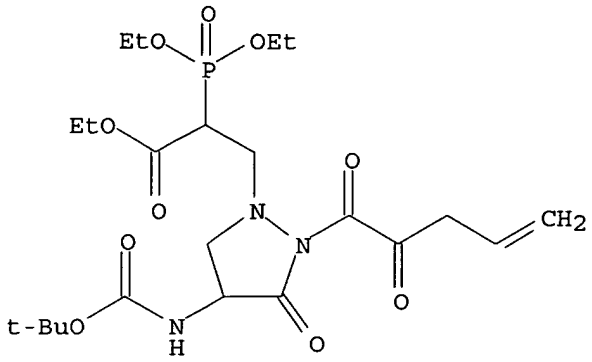
= H, C1-6 (un)substituted alkyl, perfluoro C2-4 alkyl, CCl3, etc.], CO2R9 [R9 = H, cation, C1-6 (un)substituted alkyl, etc.], PO3(R10)2 [R10 = H, cation, C1-6 (un)substituted alkyl, etc.], CH2N+.tplbond.Q (N+.tplbond.Q = quaternary ammonium group), heterocyclylthiomethyl, OR11 [R11 = H, C1-6 (un)substituted alkyl, etc.], NR12R13 [R12, R13 = H, C1-6 (un)substituted alkyl, etc.], CO2R14 (R14 = C1-6 alkyl, C7-12 arylalkyl, Ph); the other of R1, R2 = CO2R15 (R15 = cation, CO2H-protecting group, non-toxic, metabolically labile ester-forming group; R3, R4 = H, C1-6 (un)substituted alkyl, C7-12 (un)substituted arylalkyl, (un)substituted Ph, CO2R9; R5, R6 = H, amino protecting group, C1-30 acyl; at least 1 of R5, R6 = H; R5R6N = phthalimido] and their pharmaceutically acceptable salts, useful as antibacterials (no data), were prepared Me 3-hydroxy-2(S)-(tert-butoxycarbonylamino)propionate was tosylated and the product cyclocondensed with N2H4 to give 48% 4(R,S)-(tert-butoxycarbonylamino)-3-oxo-1-pyrazoline. Treatment with 37% aqueous HCHO gave the 1-methylenepyrazolidinium ylide, which underwent cycloaddn. with diallyl butynedioate to give 32.8% diallyl 7(R,S)-(tert-butoxycarbonylamino)-8-oxo-1,5-diazabicyclo[3.3.0]oct-2-ene-2,3-dicarboxylate. This was deprotected and the free amino group acylated with 2-thienylacetyl chloride to give 62% 7(R,S)-II.

IT **106892-69-7P 106892-71-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

RN 106892-69-7 CAPLUS
CN 1-Pyrazolidinepropanoic acid, α-(diethoxyphosphinyl)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-(1,2-dioxo-4-pentenyl)-3-oxo-, methyl ester (9CI) (CA INDEX NAME)



RN 106892-71-1 CAPLUS
CN 1-Pyrazolidinepropanoic acid, α-(diethoxyphosphinyl)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-(1,2-dioxo-4-pentenyl)-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)



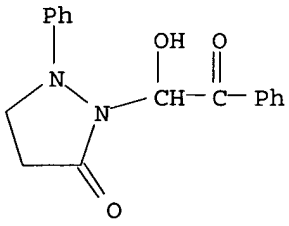
L11 ANSWER 16 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1986:543445 CAPLUS
DOCUMENT NUMBER: 105:143445
TITLE: Silver halide photographic photosensitive materials
INVENTOR(S): Ichijima, Yasushi; Sato, Shingo
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 22 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61032839	A2	19860215	JP 1984-155765	19840726
JP 05037299	B4	19930602		
PRIORITY APPLN. INFO.:			JP 1984-155765	19840726

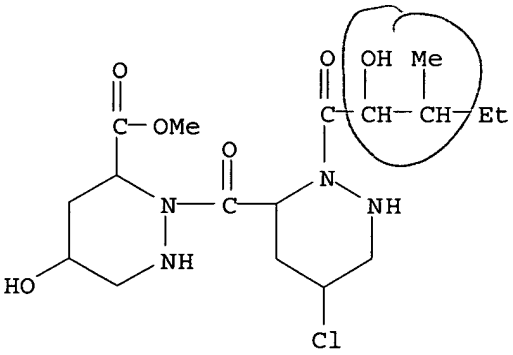
AB The claimed photog. materials contain ≥1 compound of the formula RCR1R2ZR3 [I: R = photog. useful compound moiety; R1 = H, substituent; R2 = substituent; R3 = H, a group released (from Z) in the presence of an alkali; Z = O, S, NR4 (R4 = H, substituent); two of R - R4 may combine to form a ring]. The compds. I releases photog. useful compds. (such as fog inhibitors, development promoting agent, etc.) with good timing.

IT **104367-85-3**
RL: USES (Uses)
(photog. development promoter releaser)

RN 104367-85-3 CAPLUS
CN 3-Pyrazolidinone, 2-(1-hydroxy-2-oxo-2-phenylethyl)-1-phenyl- (9CI) (CA INDEX NAME)



L11 ANSWER 17 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1978:136946 CAPLUS
DOCUMENT NUMBER: 88:136946
TITLE: Amino-acids and peptides. Part 19. Conformational studies of the monamycins, a family of cyclohexadepsipeptide antibiotics
AUTHOR(S): Hassall, Cedric H.; Thomas, W. Anthony; Moschidis, Michael C.
CORPORATE SOURCE: Roche Prod. Ltd., Welwyn Garden City, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1977), (21), 2369-76
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 1H and 13C NMR and IR spectral studies of monamycin D1 and H1 support a single all trans conformation for each congener incorporating a β-loop with H bonding of the NH groups of the valine residue to the carbonyl of the hydroxypiperazic acid residue.
IT **66008-30-8**
RL: PRP (Properties)
(NMR of)
RN 66008-30-8 CAPLUS
CN 3-Pyridazinecarboxylic acid, 2-[[5-chlorohexahydro-2-(2-hydroxy-3-methyl-1-oxopentyl)-3-pyridazinyl]carbonyl]hexahydro-5-hydroxy-, methyl ester, [3R-[2(2S*,3S*),3α(3S*,5S*),5β]]- (9CI) (CA INDEX NAME)

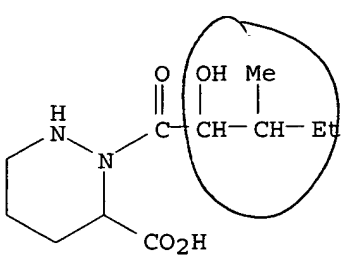


No tautomer possible

L11 ANSWER 18 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1971:112420 CAPLUS
DOCUMENT NUMBER: 74:112420
TITLE: Amino acids and peptides. XII. Molecular structures of the monamycins, cyclodepsipeptide antibiotics
AUTHOR(S): Hassall, Cedric H.; Morton, R. B.; Ogihara, Yukio; Phillips, D. A. S.
CORPORATE SOURCE: Dep. Chem., Univ. Coll. Swansea, Swansea, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (1971), (3), 526-32
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Mol. structures of monamycins D1 (I,X = H) and H1 (I, X = Cl), major constituents of a mixture of 15 related cyclohexadepsipeptides isolated from Streptomyces jamaicensis, were determined through partial hydrolysis to di- and

tripeptides and by mass spectral studies of the Me esters of the corresponding linear hexadepsipeptides. Related structures of the minor components were elucidated through mass spectrometry.

IT **31687-27-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 31687-27-1 CAPLUS
CN 3-Pyridazinecarboxylic acid, hexahydro-2-(2-hydroxy-3-methylvaleryl)-, stereoisomer (8CI) (CA INDEX NAME)

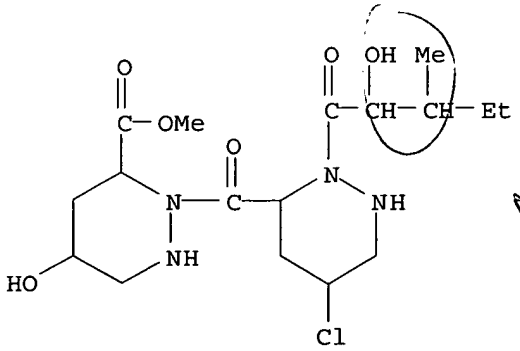


No tautomer possible

L11 ANSWER 19 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1971:99965 CAPLUS
DOCUMENT NUMBER: 74:99965
TITLE: Amino acids and peptides. XI. (3R,5S)-5-chloropiperazic acid and (3S,5S)-5-hydroxypiperazic acid, products of hydrolysis of monamycin
AUTHOR(S): Hassall, Cedric H.; Ogihara, Yukio; Thomas, William Anthony
CORPORATE SOURCE: Dep. Chem., Univ. Coll. Swansea, Swansea, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (1971), (3), 522-6
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Degradation and PMR spectra established two imino acids isolated from acid hydrolyzates of monamycin, an antibiotic of Streptomyces jamaicensis, as (3R,5S)-5-chloropiperazic acid and (3S,5S)-5-hydroxypiperazic acid. Piperazic acid is hexahydro-3-pyridazinecarboxylic acid.

IT **31460-67-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 31460-67-0 CAPLUS
CN 3-Pyridazinecarboxylic acid, 2-[[5-chlorohexahydro-2-(2-hydroxy-3-methylvaleryl)-3-pyridazinyl]carbonyl]hexahydro-5-hydroxy-, methyl ester, stereoisomer (8CI) (CA INDEX NAME)



No tautomer possible

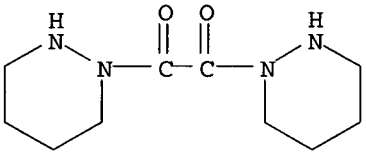
L11 ANSWER 20 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1966:93490 CAPLUS
DOCUMENT NUMBER: 64:93490
ORIGINAL REFERENCE NO.: 64:17601g-h,17602a-f
TITLE: Synthesis of completely hydrogenated dipiperidazino tetrazine, tetrazepine, and tetrazozine derivatives
AUTHOR(S): Rink, M.; Krebber, D.; Fanslau, D.; Mehta, S.
CORPORATE SOURCE: Univ. Bonn, Germany
SOURCE: Arch. Pharm. (1966), 299(3), 254-62
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 64:93490
GI For diagram(s), see printed CA Issue.
AB Piperidazine (I) with CH2O or BzH gave II (R = H) (III) and II (R = Ph) (IV), resp. 1-Carbethoxypiperidazine (V) gave similarly bis(1,1'-carbethoxy-2,2'-piperidazyl)methane (VI). I with (CO2Et)2 yielded bis(1-piperidazyl)oxamide (VII) which was reduced with LiAlH4 to 1,2-bis(1-piperidazyl)ethane (VIII). VIII was also prepared from I with (CH2Br)2. VIII was cyclized with CH2O to IX. VIII with (COCl)2 yielded X (X = O) (XI) which reduced with LiAlH4 gave X (X = H2) (XII). I (5g.), b16 56-8° [I.2HCl, m. 135-7°; bis-(phenylurea) derivative, m. 278-80°], in 200 cc. acetate buffer (pH 5.5) treated 2 days with 10 g. 35% aqueous CH2O yielded nearly quant. III, m. 167-8° (cyclohexane and petr. ether). I (5 g.) treated 15 min. at room temperature with 10 g. BzH in 100 cc. EtOH yielded nearly quant. IV, m. 245.5-6.5° (EtOH). V (5 g.), b16 113-14°, with 10 g. aqueous CH2O yielded nearly quant. VI, b0.01 150°, m. 106° (sublimed in vacuo). I (34.5 g.) in 20 cc. 9:1 cyclohexane-C6H6 treated dropwise with stirring with 58.5 g. (CO2Et)2 in 20 cc. cyclohexane-C6H6 and kept 2-3 hrs. yielded 34.4 g. 1-piperidazyloxalic acid Et ester, m. 56-7°. Na (11.5 g.) in 300 cc. absolute EtOH and 43 g. I treated dropwise with 36.5 g. (CO2Et)2 in 100 cc. absolute EtOH, refluxed 24 hrs., treated with an addnl. 18.25 g. (CO2Et)2, and again refluxed 24 hrs. gave 18.5 g. VII, m. 231-3° (C6H6). VII (18 g.) refluxed 24 hrs. with 6.1 g. LiAlH4 in 400 cc. dioxane gave 7 g. VIII, b0.2 112-13°. I (43 g.) in 40 cc. absolute Et2O and 41 g. AcONa treated dropwise with 47 g. (CH2Br)2 and stirred 24 hrs. gave 18 g. VIII, b0.2 112-13°; picrate, m. 136-8° (H2O); bis(phenylurea) derivative, m. 214-17° (40% aqueous EtOH). I (4.3 g.) treated dropwise with 4.7 g. (CH2Br)2 and stirred 4 hrs. gave VIII.2HBr, m. 227-8° (decomposition) (EtOH). VIII (5 g.) in 250 cc. acetate buffer treated with stirring during several hrs. with 5 g. 40% aqueous CH2O in 100 cc. acetate buffer and stirred 3 days yielded 1.5 g. IX, b0.1 93-5°; picrate, m. 155-7° (AcOEt). VIII (10 g.) in 400 cc. dry C6H6 and 14 g. powdered K2CO3 treated slowly with stirring and warming with 6.5 g. (COCl)2 in 50 cc. dry C6H6 and refluxed 1 hr. gave 0.85 g. XI, m. 160-1° (AcOEt-cyclohexane). XI (1.5 g.) refluxed 10 hrs. with 2 g. LiAlH4 in 100 cc. dry dioxane yielded 0.4 g. XII, b0.01 106°; picrate, m. 197° (decomposition) (60% EtOH); picrolonate, m. 226-7° (decomposition). I (17.2 g.) and 20.8 g. HOCH2CO2Et in 2:1 cyclohexane-MePh refluxed 16 hrs. yielded 12.5 g. glycolic acid piperidazide (XIII), m. 79-80° (1:1 MePh-cyclohexane). XIII (14.4 g.) in 60 cc. dry CHCl3 treated dropwise with 50 cc. SOCl2 and heated 1 hr. on the water bath gave 14.1 g. crude yellowish chloroacetic acid piperidazide HCl salt, m. 146-8° (Me2CO). HOCH2CO2Bu (132 g.) and 75 g. N2H4.H2O refluxed 2 hrs. gave quant. HOCH2CONHNH2, m. 93° (EtOH), which was converted to XIV, m. 210-11° (EtOH), in 66% yield, Rf 0.19 (30:8:3 BuOH-H2O concentrated HCl). XIV (2.9 g.) heated 2 hrs. in 50 cc. 1:3 Ac2OC5H5N gave nearly quant. the 1,5-diacetyl derivative of XIV, m. 109-11°

(iso-PrOH). XIV (14.4 g.) and 2.9 g. Na in 250 cc. refluxing absolute EtOH treated dropwise with 35 g. (CH2CO2Et)2 and refluxed 14 hrs. gave 9.1 g. yellowish-green Et succinylsuccinate, m. 126-7° (70% aqueous EtOH), Rf 0.95-1.0, and 3 g. EtO2CCH2CH2CO derivative of XIV, m. 163-4° (dioxane or Me2CO), Rf 0.19. (NHCHO)2 (8.8 g.), m. 159-60° (aqueous EtOH), in 200 cc. absolute EtOH and 100 cc. dry C6H6 stirred with warming with 4.6 g. Na to solution, treated dropwise during 8 hrs. with 18.8 g. (CH2Br)2 in 50 cc. 1:2 C6H6-EtOH, and refluxed 5 hrs. with stirring yielded 7.2 g. [CH2OCH:NN:CHONa]2, m. 244-5°.

IT **5767-22-6**, Pyridazine, 1,1'-oxalylbis[hexahydro- **6039-69-6**, Pyridazine, 1-glycoloylhexahydro-
(preparation of)

RN 5767-22-6 CAPLUS

CN Pyridazine, 1,1'-oxalylbis[hexahydro- (7CI, 8CI) (CA INDEX NAME)



RN 6039-69-6 CAPLUS

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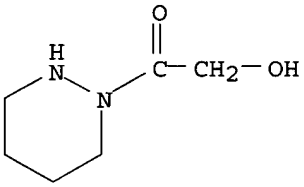


L11 ANSWER 21 OF 21 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1956:12382 CAPLUS

DOCUMENT NUMBER: 50:12382

ORIGINAL REFERENCE NO.: 50:2603g-i,2604a-c

TITLE: Dihydrophenazonyl radicals

AUTHOR(S): Wittig, Georg; Schuhmacher, Alfred

CORPORATE SOURCE: Univ. Tubingen, Germany

SOURCE: Chemische Berichte (1955), 88, 234-46
CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 50:12382

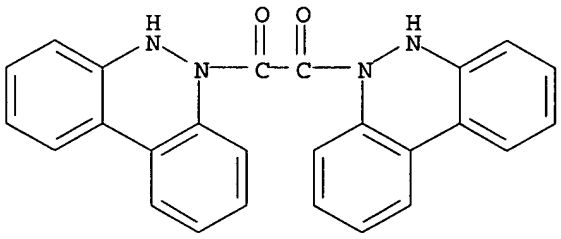
AB Addition of 6 millimoles PhLi (I) to a suspension of 1.1 g. phenazone (benzo[c]cinnoline) (II) in 20 ml. Et2O under N gave N-phenyl-N,N'-dihydrophenazone (5,6-dihydro-5-phenylbenzo[c]cinnoline) (III), m. 122-4°, unstable in air. Addition of 6 millimoles BzCl to a similar mixture of I and II gave 60% N-phenyl-N'-benzoyldihydrophenazone, m. 166-7°. Dried III (from 20 millimoles each of I and II), stirred 3 hrs. with 10 g. Ag2O in 40 ml. CHCl3, gave 36% 3-oxo-9-phenyl-3,9-dihydrophenazone [6-phenyl-benzo[c]cinnolin-2(6H)-one] (IV), orange-red needles, m. 231-2°. Treatment of 0.81 g. IV in 30 ml. Ac2O with 3

g. Zn dust yielded 78% 9-phenyl-10-acetyl-3-acetoxy-9,10-dihydrophenazone, m. 128.5°, reconverted to IV by boiling in NaOH-MeOH in air. The action of 0.3 g. Li on 0.9 g. II in 50 ml. Et2O, followed by the addition of 1.2 g. BzOH to precipitate BzOLi gave a solution of 5,6-dihydrobenzo[c]cinnoline (V), to which was added a solution of 5 millimoles acyl chloride in ether. After standing 1 hr. the mixture gave 75-91% N-acyldihydrophenazone (VI), where the acyl group is Ac, m. 113.5-14°; palmitoyl, m. 90°, hexahydrobenzoyl, m. 135.5-7.0°; crotonyl, m. 132-2.5°; and cinnamyl, m. 163-4°. Treatment of VI with the corresponding acyl chlorides in pyridine gave N,N'-diacyldihydrophenazone (VII) as follows: di-Ac (made by use of Ac2O), m. 168.5-9.5°; dipalmitoyl, m. 58-60°; bis(hexahydrobenzoyl), m. 178-9°; dicrotonyl, 192-4°; dicinnamyl, m. 289-90°; and dibenzoyl, m. 158-9°. Attempted dehydrogenation of VI with PbO2, Bz2O2, p-quinone, and Ph3C gave in each case II and the corresponding VII. Treatment of 5 millimoles N-lithiodihydrophenazonyl (from dilithiodihydrophenazone and II) with BzCl gave II and 9,10-dibenzoyl-dihydrophenazone. Interaction of 5 millimoles V and 2.5 millimoles oxalyl chloride in ether yielded 50% 9,9'-oxalylbis-(dihydrophenazone), m. 223-5° (decomposition). 9,9'-Succinoylbis(dihydrophenazone) (VII), m. 218-20° was similarly prepared, while 9,9-adipoylbis(dihydrophenazone) was made (78% yield) from adipoyl chloride and the mono-Li derivative of V. Each of the above amides gave 85-92% II on treatment with PbO2. VIII and Ph3C gave II and Ph3CH. A suspension of 0.56 g. 3,4:5,6-dibenzophenazone (IX) in 100 ml. Et2O was stirred 10 hrs. with 0.6 g. Na wire; the mixture was filtered and 0.48 g. BzOH in 10 ml. EtOH was added. To the resulting clear solution of N,N'-disodiodihydrodibenzophenazone was added 0.16 g. AcCl, giving 0.55 g. N-acetyl-N,N'-dihydro-3,4:5,6-dibenzophenazone (X), m. 121° (decomposition). Reaction of 0.65 g. X with 0.7 g. PbO2 in CHCl3 gave 0.49 g. IX. Heating of X with Ac2O gave N,N'-diacetyl-N,N'-dihydro-3,4:5,6-dibenzophenazone, also obtained by heating IX with Ac2O and Zn dust.

IT **858507-77-4**, Benzo[c]cinnoline, 5,5'-oxalylbis[5,6-dihydro- (preparation of)

RN 858507-77-4 CAPLUS

CN Benzo[c]cinnoline, 5,5'-oxalylbis[5,6-dihydro- (5CI) (CA INDEX NAME)



MARPAT (11 ~~hits~~ references) -narrower structure

Truong 09_835523 10/19/2005

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FILE CONTENT: 1988-PRESENT (VOL 143 ISS 15)(20051016/ED)

MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US    6916824 12 JUL 2005
DE 1020040544 28 JUL 2005
EP    1555012 20 JUL 2005
JP 2005191426 14 JUL 2005
WO 2005079855 01 SEP 2005

Expanded G-group definition display now available.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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L21             STR
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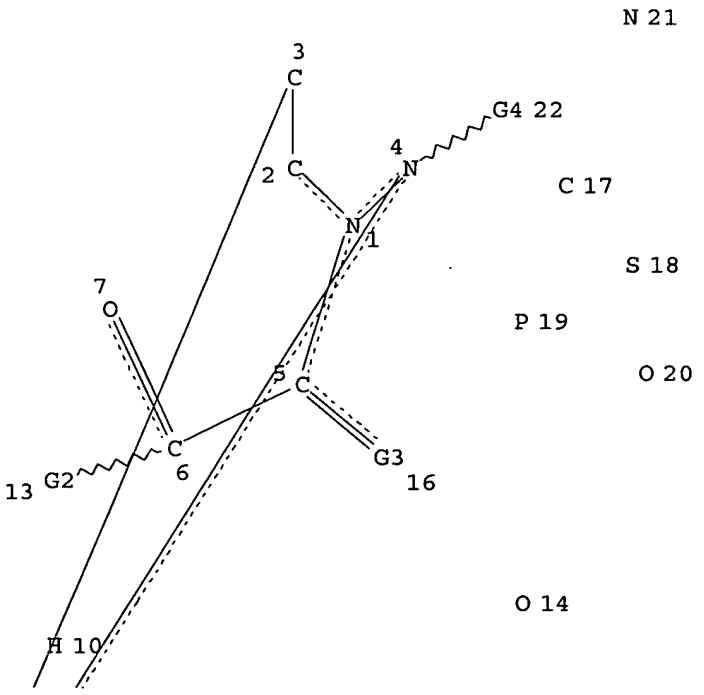

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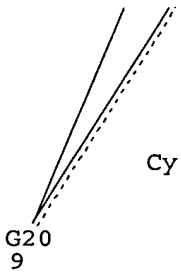

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STEREO ATTRIBUTES: NONE
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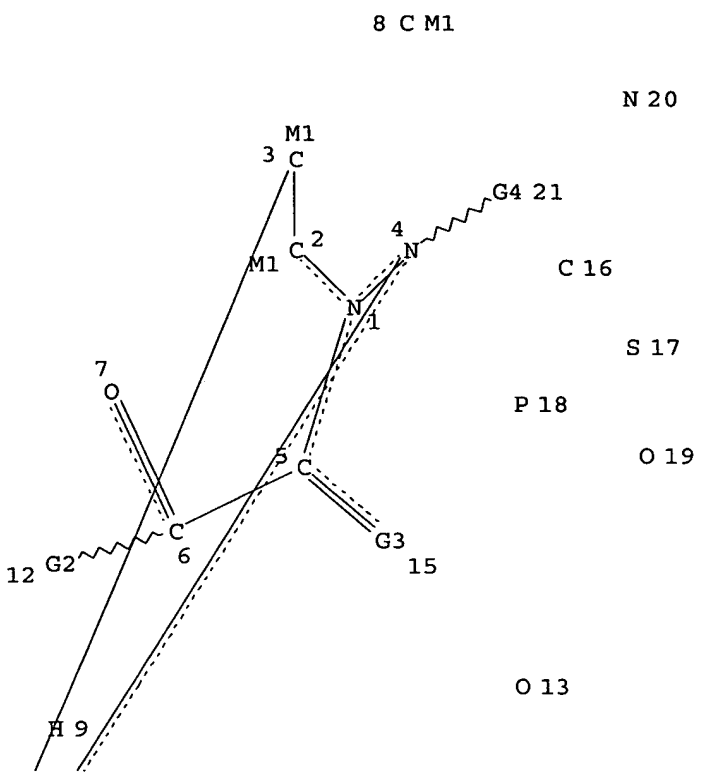

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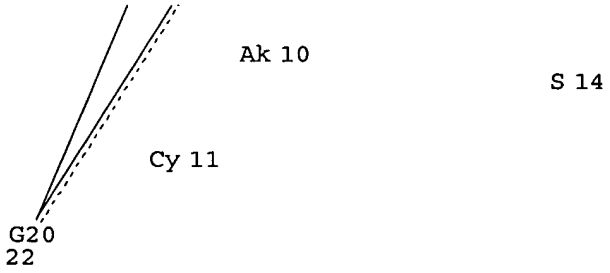

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NUMBER OF NODES IS  22

STEREO ATTRIBUTES: NONE
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L41  ANSWER 22 OF 32  MARPAT  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:        139:180074  MARPAT
TITLE:                   New pyridazine derivatives active as inhibitors of
                         cathepsin K, their pharmaceutical compositions, and
                         their preparation process
INVENTOR(S):             Bhatnagar, Neerja; Benard, Didier; Gourvest, Jean
```

Answers 1-21 previously printed

Answers 22-32 begin here

Francois; Mauger, Jacques
PATENT ASSIGNEE(S): Aventis Pharma S.A., Fr.
SOURCE: Fr. Demande, 53 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2835835	A1	20030815	FR 2002-1632	20020211
FR 2835835	B1	20040416		
CA 2475439	AA	20030821	CA 2003-2475439	20030207
WO 2003068140	A2	20030821	WO 2003-FR381	20030207
WO 2003068140	A3	20040408		
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EP 1476434	A2	20041117	EP 2003-717380	20030207
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JP 2005525334	T2	20050825	JP 2003-567325	20030207
US 2005165017	A1	20050728	US 2004-916175	20040811
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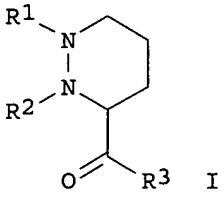
			WO 2003-FR381	20030207

GI



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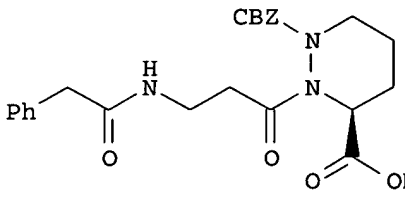

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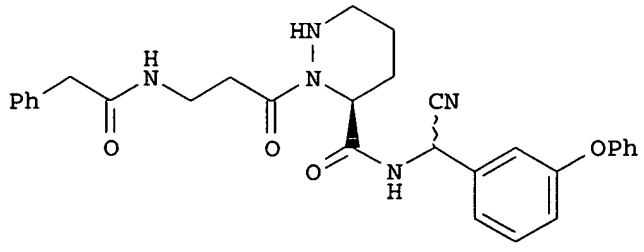

III

AB The invention discloses compds. I [in which R1 = H, alkyl, COR, COOR; R = alkyl, pyridylalkyl, carbamoylalkyl, alkenylmethyl, (un)substituted aryl or aralkyl; R2 = CO(CH2)nX with optional double bond when n = 2 or 3; n = 0-3; X = (un)saturated mono- or bicyclic heterocycle, (un)substituted aryl or aralkyl, NR4R5, COR; R4 = alkyl, COR, CONHR, CSNHR, SO2R; R5 = H or alkyl; R3 = -Y(CH2)mC(CN)R6R7; Y = O or NR8; R8 = H, alkyl; m = 0-3; R6 = H, alkyl, (un)substituted aryl or aralkyl; R7 = H or alkyl; or R6R7 forms a saturated 6-membered ring; including all stereoisomers and acid or base salts]. The compds. are useful for treating diseases associated with metabolic enzymes, specifically proteases and kinases, and particularly cathepsin K. Examples include prepns. of approx. 25 compds. I, and various intermediates. For instance, amidation β-alanine with PhCH2COCl in the presence of NaOH gave 94.2% PhCH2CONHCH2CH2CO2H. This acid was activated with oxalyl chloride and coupled with the corresponding tetrahydropyridazine derivative to give intermediate II in 26% yield. Saponification of II (84%), amidation of the resultant acid with 3-PhOC6H4CH(NH2)CN using EDCI and HOBT (50%), and hydrogenolysis of the CBZ group (67%), gave title compound III. This compound inhibited cathepsin K in vitro with an IC50 value < 1 μM.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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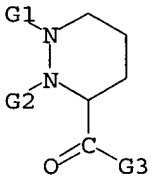

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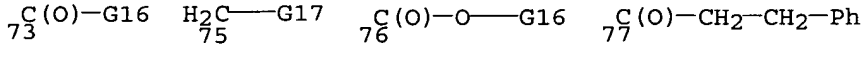
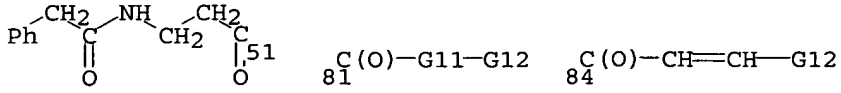
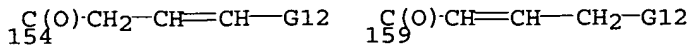
heteroaryl <containing zero or more N, zero or more O, zero or more S (no other heteroatoms), 5 or more C> (opt. substd. by 1 or more G18) /
alkyl <containing 1-5 C> (substd. by 1 or more G10) /
(Specifically claimed: Me / CH2Ph / CO2CH2Ph / 77)



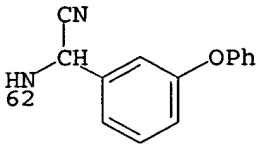
G2 = **81** / 84 / 154 / 159 / (Specifically claimed: 51)

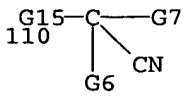


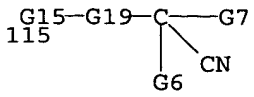


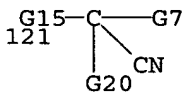
G3 = 110 / 115 / 121 / 126 / 132 / 136 / OH /

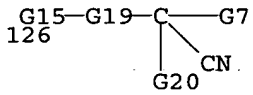
alkoxy <containing 1-6 C> / (Specifically claimed: 62) /
(Example: OMe)

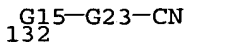


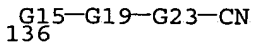




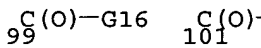


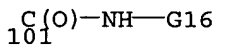


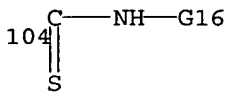


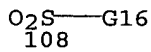


G4 = alkyl <containing 1-6 C> / 99 / 101 / 104 / 108

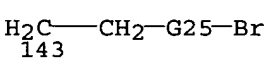




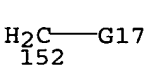




G5 = alkyl <containing 1-6 C>
G6 = H / aryl (opt. substd. by G21) /
heteroaryl <containing zero or more N, zero or more O,
zero or more S (no other heteroatoms), 5 or more C>
(opt. substd. by G21) / aryl <containing 6-10 C>
(substd. by alkyl <containing 1 or more C>) /
heteroaryl <containing zero or more N, zero or more O,
zero or more S (no other heteroatoms), 5 or more C>
(substd. by alkyl <containing 1 or more C>) /
(Specifically claimed: Ph (opt. substd. by (1) G24) / 143)

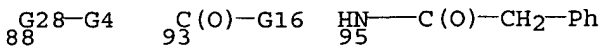


G7 = alkyl <containing 1-6 C>
G8 = H / alkyl <containing 1-6 C>
G9 = pyridyl / CONH2 / 152 /
aryl <containing 6-10 C> (opt. substd.) /
heteroaryl <containing zero or more N, zero or more O,
zero or more S (no other heteroatoms), 5 or more C>
(opt. substd.)

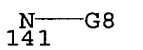


G10 = aryl <containing 6-10 C>
(opt. substd. by 1 or more G18) /
heteroaryl <containing zero or more N, zero or more O,
zero or more S (no other heteroatoms), 5 or more C>
(opt. substd. by 1 or more G18)
G11 = (0-3) CH2
G12 = heterocycle <containing 5-12 atoms, zero or more N,
zero or more O, zero or more S (no other heteroatoms),
mono- or bicyclic> / aryl <containing 6-10 C>

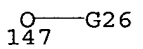
(opt. substd. by 1 or more G13) /
heteroaryl <containing zero or more N, zero or more O,
zero or more S (no other heteroatoms), 5 or more C>
(opt. substd. by 1 or more G13) /
alkyl <containing 1-5 C> (substd. by 1 or more G14) / 88 /
93 / (Specifically claimed: Ph / 95 / morpholino)



G13 = OH / NH2 / NO2 / alkyl <containing 1-6 C> /
alkoxy <containing 1-6 C> / halo
G14 = aryl <containing 6-10 C>
(substd. by 1 or more G13) / heteroaryl <containing zero or
more N, zero or more O, zero or more S (no other heteroatoms)
, 5 or more C> (opt. substd. by 1 or more G13)
G15 = O / S / 141



G16 = **alkyl <containing 1 or more C> (opt. substd. by G9)**
G17 = alkenyl <containing 3-9 C>
G18 = OH / NH2 / NO2 / alkyl <containing 1-6 C> /
alkoxy <containing 1-6 C> / halo
G19 = (1-3) CH2
G20 = alkyl <containing 1-6 C>
(opt. substd. by 1 or more G22)
G21 = OH / NH2 / NO2 / alkyl <containing 1-6 C> /
alkoxy <containing 1-6 C> (opt. substd. by G27) / 147



G22 = aryl (opt. substd. by G21)
G23 = carbocycle <containing 6 C, attached through 1 C>
(opt. substd.) / 140

G24 = H / OPh
G25 = phenylene
G26 = aryl <containing 6-11 C>
(opt. substd. by (1-3) halo) / heteroaryl <containing zero
or more N, zero or more O, zero or more S (no other
heteroatoms), 5 or more C> (substd. by (1-3) halo)
G27 = aryl <containing 6-11 C>
(opt. substd. by (1-3) halo) / heteroaryl <containing zero
or more N, zero or more O, zero or more S (no other
heteroatoms), 5 or more C> (substd. by (1-3) halo)
G28 = NH / 90

N---G5
90

Patent location: claim 1
Note: combined w/ claim 21, formula IV and claim 22, formula III
Note: and acid or base addition salts
Note: also incorporates claim 21, formula IV and claim 22, formula III
Stereochemistry: or isomer forms, racemics, enantiomers and diastereisomers

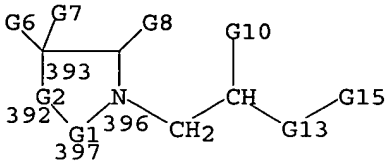
L41 ANSWER 23 OF 32 MARPAT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 131:106817 MARPAT
TITLE: Prodrugs of aspartyl protease inhibitors for treatment of HIV infections
INVENTOR(S): Hale, Michael R.; Tung, Roger D.; Baker, Christopher T.; Spaltenstein, Andrew; Furfine, Eric Steven; Kaldor, Istvan; Kazmierski, Wieslaw Mieczyslaw
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 120 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9933795	A1	19990708	WO 1998-US27510	19981224
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9920121	A1	19990719	AU 1999-20121	19981224
PRIORITY APPLN. INFO.:			US 1997-70309P	19971224
			WO 1998-US27510	19981224

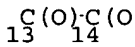
AB Prodrugs of a class of sulfonamides which are HIV aspartyl protease inhibitors are described. The prodrugs are characterized by favorable aqueous solubility, high oral bioavailability and facile in vivo generation of the active ingredient. The prodrugs and pharmaceutical compns. of this invention are particularly well suited for decreasing the pill burden and increasing patient compliance in HIV infections. E.g., a pharmaceutical composition, in addition to a prodrug, may comprise an antiviral agent, a HIV protease inhibitor other than a compound of this invention, and an immunostimulant.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

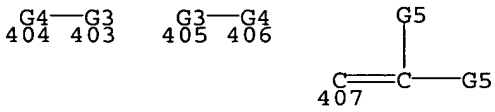
MSTR 1A



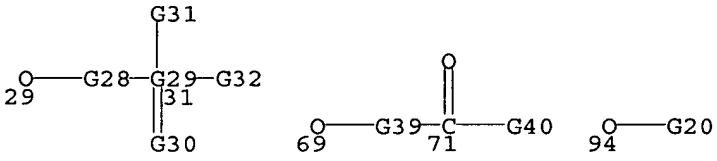
G1 = C(O) / SO2 / 13-392 14-396 / S(O)



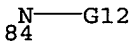
G2 = CH2 / CH2CH2 / NH (opt. substd.) /
404-393 403-397 / 405-393 406-397 / 407



G3 = NH (opt. substd.) / O / S / S(O) / SO2
G4 = (1-2) CH2
G5 = H / R
G6 = H / OH
G7 = H / OH
G8 = H / aryl (opt. substd.) /
carbocycle <containing 3 or more C> (opt. substd.) /
heterocycle <containing 1-4 heteroatoms, zero or more N,
zero or more S, zero or more O (no other heteroatoms)>
(opt. substd.) / alkyl <containing 1-6 C> (opt. substd.) /
alkenyl <containing 2-6 C> (opt. substd.) /
alkynyl <containing 2-6 C> (opt. substd.) /
cycloalkyl <containing 3-6 C> (opt. substd.) /
cycloalkenyl <containing 5-6 C> (opt. substd.)
G10 = 29 / 69 / (Specifically claimed: 94)

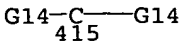


G11 = O / S / NH / 84

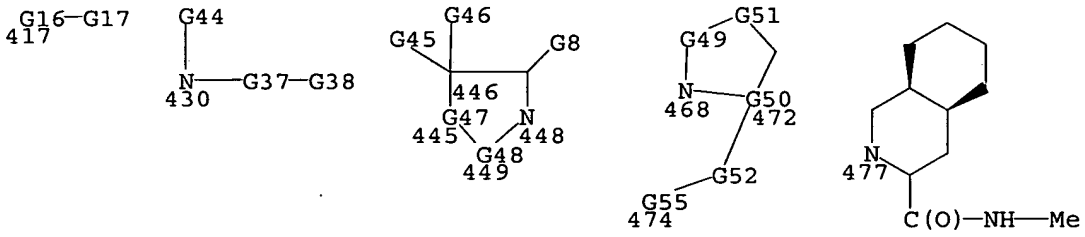


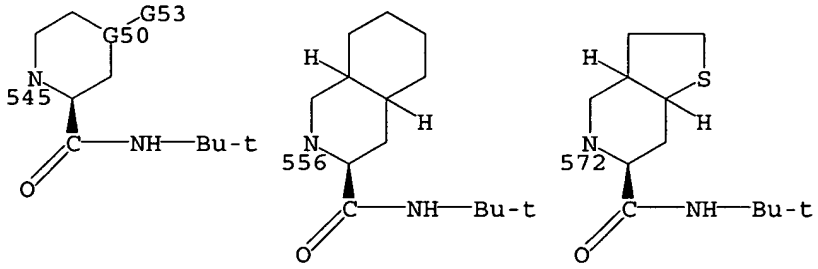
G12 = alkyl <containing 1-12 C> (opt. substd.) /
alkenyl <containing 2-12 C> (opt. substd.) /
carbocycle <containing 3 or more C> (opt. substd.) /
aryl (opt. substd.) / heterocycle <containing 1-4
heteroatoms, zero or more N, zero or more S,
zero or more O (no other heteroatoms)> (opt. substd.) /

alkynyl <containing 2-6 C> (opt. substd.) / R
G13 = **(1-2) 415**

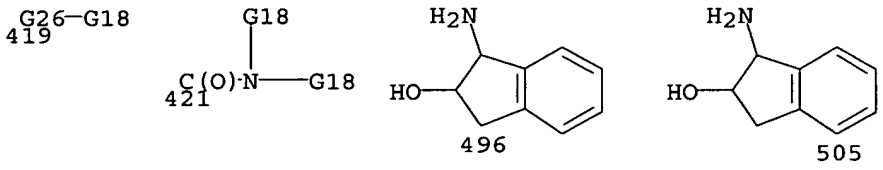


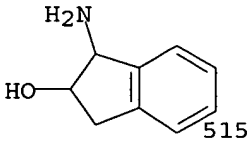
G14 = H / OH / R
G15 = 417 / 430 / 448 / **468** / (Specifically claimed: 477 / 545 / 556 / 572)





G16 = S(O) / SO2
G17 = 419 / 588 / 421 / aryl (opt. substd.) / carbocycle <containing 3 or more C> (opt. substd.) / aryl (opt. substd.) / heterocycle <containing 1-4 heteroatoms, zero or more N, zero or more S, zero or more O (no other heteroatoms)> (opt. substd.) / alkyl <containing 1-6 C> (opt. substd.) / alkenyl <containing 2-4 C> (opt. substd.) / cycloalkyl <containing 3-6 C> (opt. substd.) / cycloalkenyl <containing 5-6 C> (opt. substd.) / (Specifically claimed: 496 / 505 / 515 / 524 / 536)

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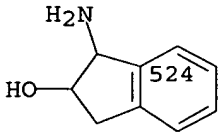
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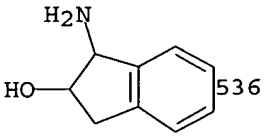
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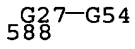
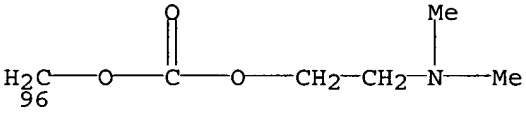

588

G18 = H / alkyl (opt. substd. by 1 or more G19) / alkenyl / alkynyl / aryl (opt. substd.) / carbocycle <containing 3 or more C> (opt. substd.) / heterocycle <containing 1-4 heteroatoms, zero or more N, zero or more S, zero or more O (no other heteroatoms)> (opt. substd.)

G19 = aryl (opt. substd.) / carbocycle <containing 3 or more C> (opt. substd.) / heterocycle <containing 1-4 heteroatoms, zero or more N, zero or more S, zero or more O (no other heteroatoms)> (opt. substd.)

G20 = 96 / 114 / 115 / 121 / 125 / 129 / 131 / 138 / 152 / 153 / 156 / 161 / 172 / 175 / 186 / 189 / 198 / 210 / 219 / COMe / COCH2Me / 220 / 236 / CHO / COCF3 / 273 / 275 / 282 / 292 / 294 / 296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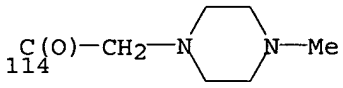
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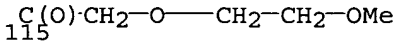
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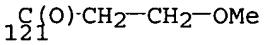
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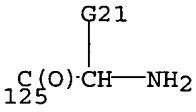
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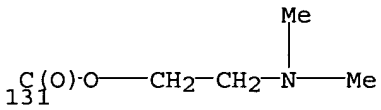
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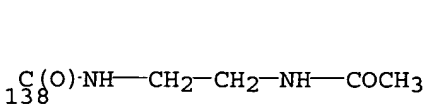
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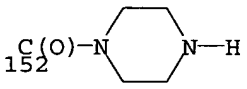
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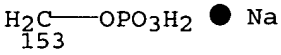
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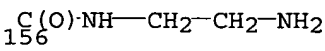
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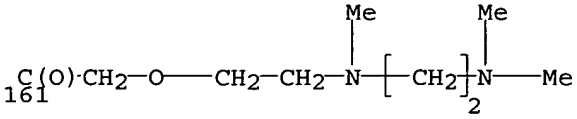
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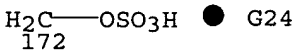
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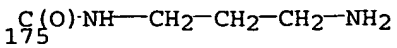
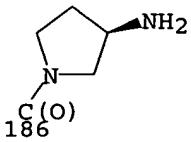
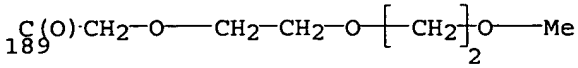
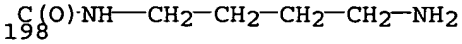
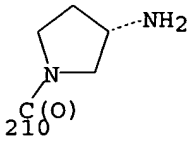
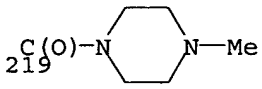


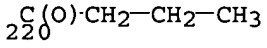


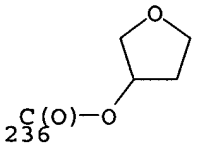


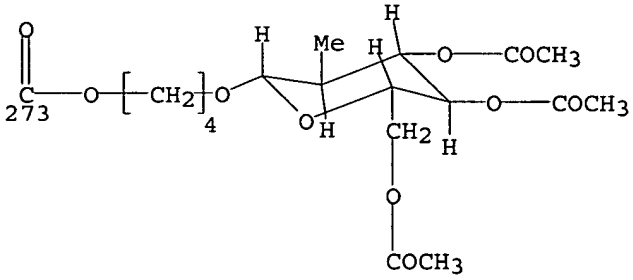


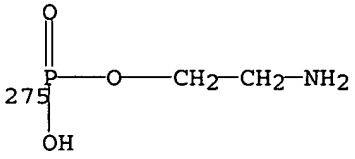


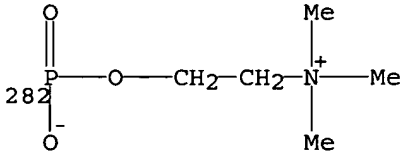


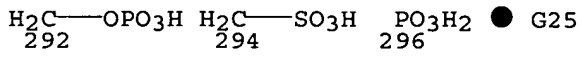






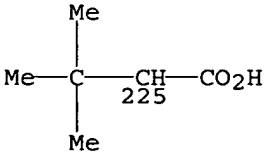


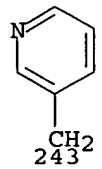


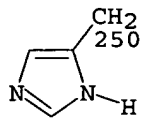


● G25

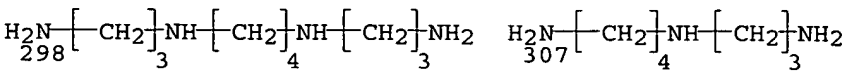
G21 = CH2CH2CH2CH2NH2 / CH2C6H4OH-p / CH2OH / Pr-i / CH2CH2CO2H / CH2CO2H / 225 / 243 / 250



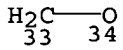




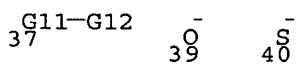
G22 = Na / Mg / NH3
G23 = PO3H2 / SO3H
G24 = Na / NH3
G25 = K / Ca / 298 / 307



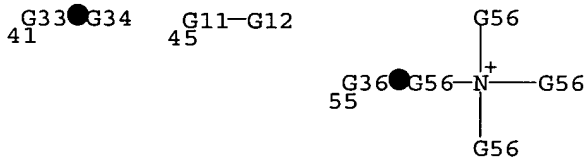
G26 = O / NH (opt. substd.) / S(O) / SO2
G27 = (1-2) C(O)
G28 = bond / 33-29 34-31



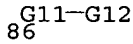
G29 = P / S
G30 = O / S
G31 = OH / SH / NH2 / 37 / 39 / 40 / H



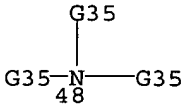
G32 = OH / SH / NH2 / 45 / 41 / 55 / H



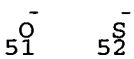
G33 = OH / SH / NH2 / 86



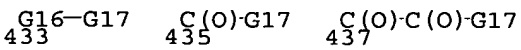
G34 = Li / Na / K / Mg / Ca / Ba / 48



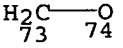
G35 = H / alkyl <containing 1-4 C> (opt. substd.)
G36 = 51 / 52



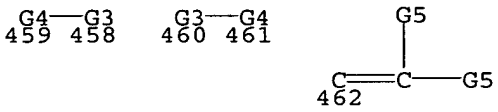
G37 = bond / NH (opt. substd.) / CH2 (opt. substd.)
G38 = 433 / 435 / 437



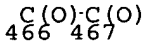
G39 = bond / 73-69 74-71



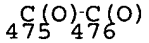
G40 = H / alkyl <containing 1-12 C> (opt. substd.) /
alkenyl <containing 2-12 C> (opt. substd.) /
carbocycle <containing 3 or more C> (opt. substd.) /
aryl (opt. substd.) / heterocycle <containing 1-4
heteroatoms, zero or more N, zero or more O,
zero or more S (no other heteroatoms)> (opt. substd.) / R
G44 = H / R
G45 = H / OH
G46 = H / OH
G47 = CH2 / CH2CH2 / NH (opt. substd.) /
459-446 458-449 / 460-446 461-449 / 462



G48 = C(O) / SO2 / 466-445 467-448 / S(O)



G49 = **(1-3) CH2**
G50 = CH / **N**
G51 = NH (opt. substd.) / O / S / S(O) / SO2 / C(O) /
CH2 (opt. substd.)
G52 = C(O) / SO2 / **475-474 476-472** / S(O)



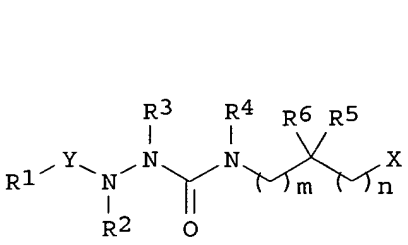
G53 = H / alkyl <containing 1-6 C> (opt. substd.) /
alkenyl <containing 2-6 C> (opt. substd.) /
alkynyl <containing 2-6 C> (opt. substd.) /
cycloalkyl <containing 3-6 C> (opt. substd.) /
cycloalkenyl <containing 5-6 C> (opt. substd.) / R
G54 = H / carbon chain <0 or more double bonds,
0 or more triple bonds> (opt. substd.) /
carbocycle <containing 3 or more C> (opt. substd.) /
heterocycle <containing 1-4 heteroatoms, zero or more N,
zero or more S, zero or more O (no other heteroatoms)>
(opt. substd.)
G55 = R / aryl (opt. substd.) /
carbocycle <containing 3 or more C> (opt. substd.) /
heterocycle <containing 1-4 heteroatoms, zero or more N,
zero or more S, zero or more O (no other heteroatoms)>
(opt. substd.) / **alkyl <containing 1-6 C> (opt. substd.)** /
alkenyl <containing 2-4 C> (opt. substd.) /
cycloalkyl <containing 3-6 C> (opt. substd.) /
cycloalkenyl <containing 5-6 C> (opt. substd.)

G56 = alkyl <containing 1-4 C> (opt. substd.)
G6 +G7 = O
G45+G46= O
Patent location: claim 1
Note: substitution is restricted
Note: additional oxo formation and ring formation also claimed

L41 ANSWER 24 OF 32 MARPAT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 130:282371 MARPAT
TITLE: Preparation of azapeptide acids as cell adhesion inhibitors
INVENTOR(S): Delaszlo, Stephen E.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 94 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9920272	A1	19990429	WO 1998-US22008	19981019
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6069163	A	20000530	US 1998-174631	19981016
AU 9913614	A1	19990510	AU 1999-13614	19981019
PRIORITY APPLN. INFO.:			US 1997-62874P	19971021
			US 1997-65763P	19971117
			GB 1997-24874	19971126
			WO 1998-US22008	19981019

GI



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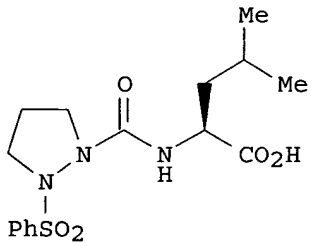


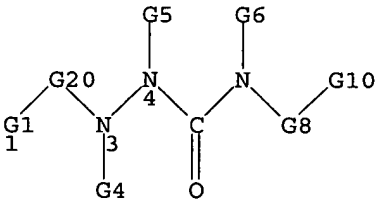
II

AB Azapeptide acids I [(un)substituted C1-10 alkyl, C2-10 alkenyl, C2-10 alkynyl, Cy, Cy-C1-10 alkyl, Cy-C2-10 alkenyl, Cy-C2-10 alkynyl; R2, R3 = independently H, any group R1; R2R3 form (un)substituted, optionally benzo-fused 4-7-membered heterocyclic ring; R5 = H, (un)substituted C1-10 alkyl, C2-10 alkenyl, C2-10 alkynyl, aryl, aryl-C1-10 alkyl, heteroaryl, heteroaryl-C1-10 alkyl; R6 = H, (un)substituted Ar1-Ar2-C1-10 alkyl,

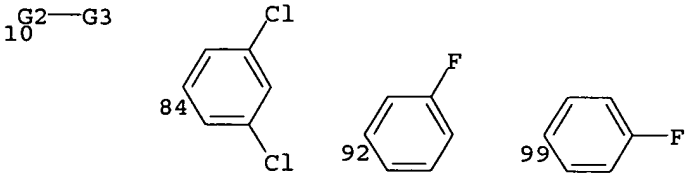
Ar1-Ar2-C2-10 alkenyl, Ar1-Ar2-C2-10 alkynyl, Ar1-C.tplbond.C-Ar2-C1-10 alkyl,Ar1-C2 alkenyl-Ar2-C1-10 alkyl, Ar1-Ar2, any group R1; X = CO2R8, P(O)(OR8)(OR9), SOmOR8, CONR9R10, 5-tetrazolyl, CONHSO2R11; R8, R9 = independently H, (un)substituted C1-10 alkyl, C2-10 alkenyl, C2-10 alkynyl, Cy, Cy-C1-10 alkyl; R10 = H, (un)substituted C1-10 alkyl, C2-10 alkenyl, C2-10 alkynyl, CN, aryl, , aryl-C1-10 alkyl, heteroaryl, heteroaryl-C1-10 alkyl, SO2R11; R11 = (un)substituted C1-10 alkyl, C2-10 alkenyl, C2-10 alkynyl, aryl; Y = CO, O2C, NR9CO, SO2, P(O)(OR8), COCO; Cy = cycloalkyl, heterocyclyl, aryl, heteroaryl; m = 0-2; n = 0-2], and pharmaceutically acceptable salts thereof, are antagonists of VLA-4 and/or α4β7, and as such are useful in the inhibition or prevention of cell adhesion and cell-adhesion mediated pathologies. These compds. may be formulated into pharmaceutical compns. and are suitable for use in the treatment of asthma, allergies, inflammation, multiple sclerosis, and other inflammatory and autoimmune disorders. Thus, sequential coupling of 1-(benzyloxycarbonyl)pyrazolidine (preparation given) with triphosgene and L-leucine tert-Bu ester, followed by hydrogenolysis, sulfonylation with PhSO2Cl, and acidic deesterification, gave desired free azapeptide II.

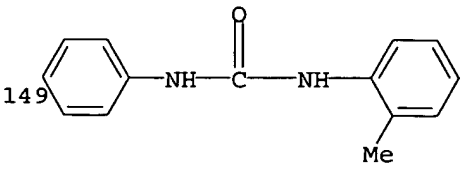
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

MSTR 1



G1 = **alkyl <containing 1-10 C> (opt. substd.) /** alkenyl <containing 2-10 C> (opt. substd.) / alkynyl <containing 2-10 C> (opt. substd.) / cycloalkyl (opt. substd.) / heterocycle <non-aromatic> (opt. substd.) / aryl (opt. substd.) / heteroaryl (opt. substd.) / 10 / (Specifically claimed: 84 / 92 / 99 / 149)





G2 = alkylene <containing 1-10 C> (opt. substd.) /

alkenylene <containing 2-10 C> (opt. substd.) /
alkynylene <containing 2-10 C> (opt. substd.)

G3 = cycloalkyl (opt. substd.) /
heterocycle <non-aromatic> (opt. substd.) /
aryl (opt. substd.) / heteroaryl (opt. substd.)

G4 = H / alkyl <containing 1-10 C> (opt. substd.) /
alkenyl <containing 2-10 C> (opt. substd.) /
alkynyl <containing 2-10 C> (opt. substd.) /
cycloalkyl (opt. substd.) / heterocycle <non-aromatic>
(opt. substd.) / aryl (opt. substd.) /
heteroaryl (opt. substd.) / 21

G2—G3
21

G5 = H / alkyl <containing 1-10 C> (opt. substd.) /
alkenyl <containing 2-10 C> (opt. substd.) /
alkynyl <containing 2-10 C> (opt. substd.) /
cycloalkyl (opt. substd.) / heterocycle <non-aromatic>
(opt. substd.) / aryl (opt. substd.) /
heteroaryl (opt. substd.) / 23 / (Specifically claimed: Pr-i)

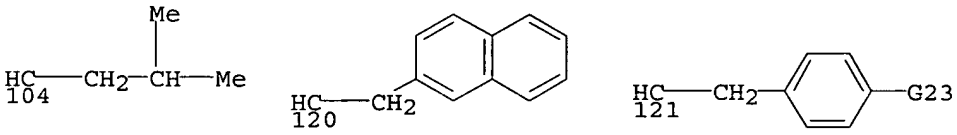
G2—G3
23

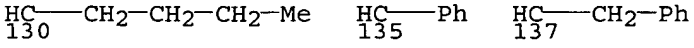
G6 = H / alkyl <containing 1-10 C> /
cycloalkyl (opt. substd.) / heterocycle <non-aromatic>
(opt. substd.) / aryl (opt. substd.) /
heteroaryl (opt. substd.) / 26

G7—G3
26

G7 = alkylene <containing 1-10 C>

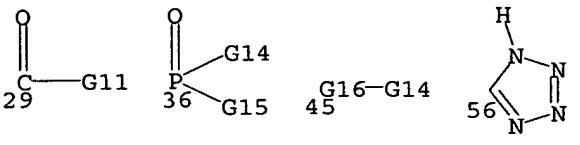
G8 = carbon chain <containing 1 or more C,
0 or more double bonds, 0 or more triple bonds>
(opt. substd. by (up to 2) G9) / G22 /
(Specifically claimed: 104 / 120 / 121 / 130 / 135 / CHMe /
137)



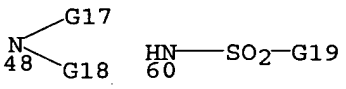


G9 = aryl (opt. substd.) / heteroaryl (opt. substd.) /
cycloalkyl (opt. substd.) / heterocycle <non-aromatic>
(opt. substd.)

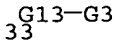
G10 = 29 / 36 / 45 / 56



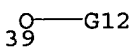
G11 = OH / 31 / 48 / 60



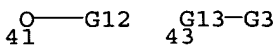
G12 = alkyl <containing 1-10 C> (opt. substd.) /
alkenyl <containing 2-10 C> (opt. substd.) /
alkynyl <containing 2-10 C> (opt. substd.) /
aryl (opt. substd.) / heteroaryl (opt. substd.) /
cycloalkyl (opt. substd.) / heterocycle <non-aromatic>
(opt. substd.) / 33



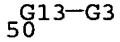
G13 = alkylene <containing 1-10 C> (opt. substd.)
G14 = OH / 39



G15 = OH / 41 / H / alkyl <containing 1-10 C>
(opt. substd.) / alkenyl <containing 2-10 C> (opt. substd.) /
alkynyl <containing 2-10 C> (opt. substd.) /
aryl (opt. substd.) / heteroaryl (opt. substd.) /
cycloalkyl (opt. substd.) / heterocycle <non-aromatic>
(opt. substd.) / 43

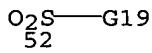


G16 = S / S(O) / SO2
G17 = H / alkyl <containing 1-10 C> (opt. substd.) /
alkenyl <containing 2-10 C> (opt. substd.) /
alkynyl <containing 2-10 C> (opt. substd.) /
aryl (opt. substd.) / heteroaryl (opt. substd.) /
cycloalkyl (opt. substd.) / heterocycle <non-aromatic>
(opt. substd.) / 50

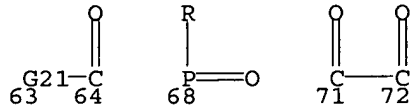


G18 = H / alkyl <containing 1-10 C> (opt. substd.) /
alkenyl <containing 2-10 C> (opt. substd.) /
alkynyl <containing 2-10 C> (opt. substd.) / CN /

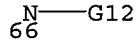
aryl (opt. substd.) / alkyl <containing 1-10 C>
(substd. by aryl (opt. substd.)) /
heteroaryl (opt. substd.) / alkyl <containing 1-10 C>
(substd. by heteroaryl (opt. substd.)) / 52



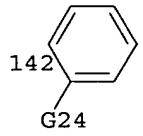
G19 = alkyl <containing 1-10 C> (opt. substd.) /
alkenyl <containing 2-10 C> (opt. substd.) /
alkynyl <containing 2-10 C> (opt. substd.) /
aryl (opt. substd.)
G20 = C(O) / 63-1 64-3 / SO2 / 68 / **71-1 72-3**



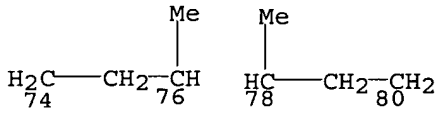
G21 = O / NH / 66



G22 = (1-5) CH2
G23 = F / Ph / 142



G24 = CN / OMe
G4 +G5 = R <"moiety necessary to complete a ring"> /
(Specifically claimed: CH2CH2CH2 (opt. substd.) /
CH2CH2CH2CH2 (opt. substd.) / 74-3 76-4 / 78-3 80-4)



Derivative: or pharmaceutically acceptable salts
Patent location: claim 1
Stereochemistry: 120,121,130-S

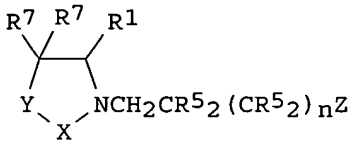
L41 ANSWER 25 OF 32 MARPAT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 131:185247 MARPAT
TITLE: Preparation of heterocyclylhydroxyalkanamides and related compounds as aspartyl protease inhibitors
INVENTOR(S): Tung, Roger Dennis; Salituro, Francesco Gerald; Deininger, David D.; Bhisetti, Govinda Rao; Baker,

Christopher Todd; Spaltenstein, Andrew
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: U.S., 69 pp., Cont.-in-part of U.S. Ser. No. 592,777.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5945413	A	19990831	US 1996-724563	19960930
US 5883252	A	19990316	US 1996-592777	19960126
CA 2243121	AA	19970731	CA 1997-2243121	19970122
WO 9727180	A1	19970731	WO 1997-US1610	19970122
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9717580	A1	19970820	AU 1997-17580	19970122
AU 709239	B2	19990826		
EP 882022	A1	19981209	EP 1997-904911	19970122
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9707086	A	19990413	BR 1997-7086	19970122
JP 2000501111	T2	20000202	JP 1997-527124	19970122
ZA 9700613	A	19970730	ZA 1997-613	19970124
AP 844	A	20000609	AP 1997-961	19970124
W: BW, GM, GH, KE, LS, MW, SD, SZ, UG, ZM, ZW				
NO 9803435	A	19980921	NO 1998-3435	19980724

PRIORITY APPLN. INFO.: US 1996-592777 19960126
US 1996-724563 19960930
WO 1997-US1610 19970122

GI



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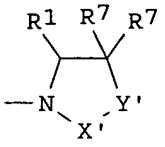
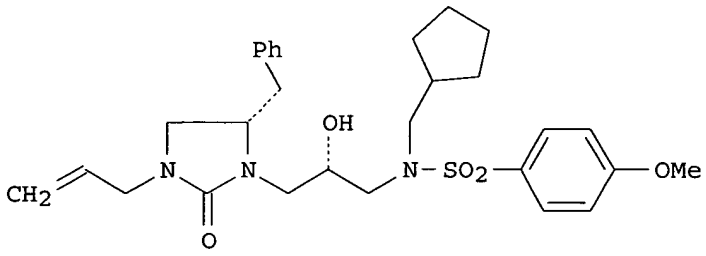


II

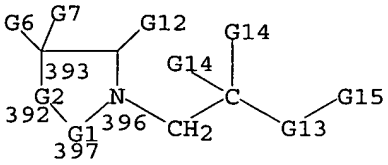


III

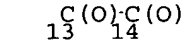
AB Title compds. I [Z = (Q)rR1X'R4, fragment II, etc., which may be fused with R6; X, X' = CO, COCO, SO, SO2; Y, Y' = (CR22)p, NR2, (CR22)pM, NR2CH2; Q = CH, N; R1, R2 = H, R6, alkyl, alkenyl, alkynyl, (fused) cycloalkyl, cycloalkenyl, etc.; R4 = (substituted) OR9, XR9, NR92, R6, alkyl, alkenyl, (fused) cycloalkyl, cycloalkenyl, etc.; R5 = H, OH, O, R1; R6 = (substituted) aryl, carbocyclyl, heterocyclyl; R7 = H, OH, O; R9 = H, alkyl, alkenyl, alkynyl, aryl, carbocyclyl, heterocyclyl, aralkyl, carbocyclylalkyl, heterocyclylalkyl; M = NH, NR2, O, S, SO, SO2; n = 1, 2; r = 0-2] were prepared for use as aspartyl protease inhibitors. Thus, compound II (preparation given) inhibited HIV aspartyl protease with Ki = 160 nM.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

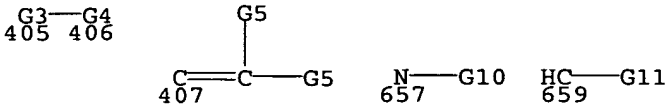
MSTR 1A



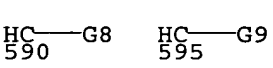
G1 = C(O) / SO2 / 13-392 14-396 / S(O)



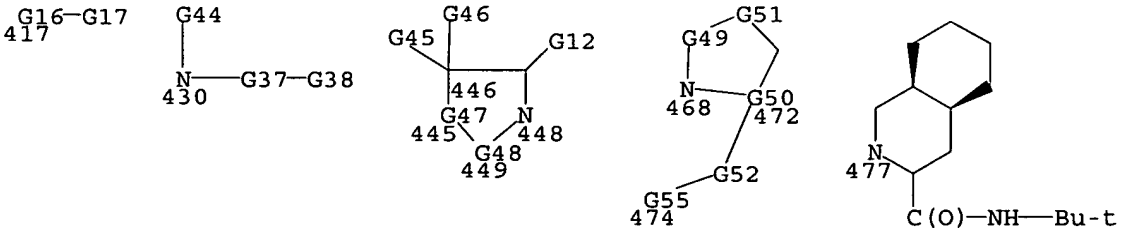
G2 = 659 / CH2CH2 / 657 / 405-393 406-397 / 407

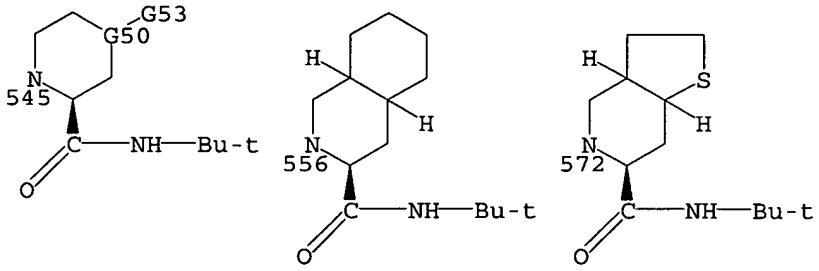


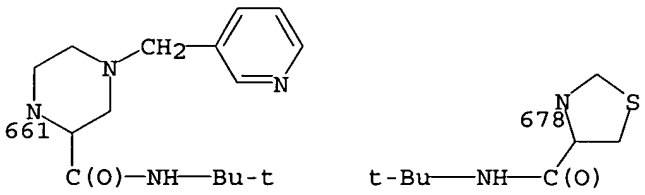
G3 = NH (opt. substd.) / O / S / S(O) / SO2
G4 = (1-2) CH2
G5 = H / R
G6 = H / OH
G7 = H / OH
G8 = H / aryl (opt. substd.) / carbocycle <containing 3 or more C> (opt. substd.) / heterocycle <containing 1-4 heteroatoms, zero or more N, zero or more S, zero or more O (no other heteroatoms)> (opt. substd.) / cycloalkyl <containing 3-6 C> (opt. substd.) / cycloalkenyl <containing 5-6 C> (opt. substd.)
G9 = carbon chain <containing 1-6 C, 0 or more double bonds, 0 or more triple bonds> (opt. substd.) / (Specifically claimed: CH2Ph (opt. substd. by G58))
G10 = H / R / (Specifically claimed: CH2CH=CH2 / CH2Ph)
G11 = H / R / (Specifically claimed: CH2CH=CH2 / CH2Ph / CH2CONH2)
G12 = H / aryl (opt. substd.) / carbocycle <containing 3 or more C> (opt. substd.) / heterocycle <containing 1-4 heteroatoms, zero or more N, zero or more S, zero or more O (no other heteroatoms)> (opt. substd.) / cycloalkyl <containing 3-6 C> (opt. substd.) / cycloalkenyl <containing 5-6 C> (opt. substd.) / carbon chain <containing 1-6 C, 0 or more double bonds, 0 or more triple bonds> (opt. substd.) / (Specifically claimed: CH2Ph (opt. substd. by G58))
G13 = G20 / (Specifically claimed: 590 / 595 / C(O))



G14 = H / OH / R
G15 = 417 / 430 / 448 / **468** / (Specifically claimed: 477 / 545 / 556 / 572 / 661 / 678)

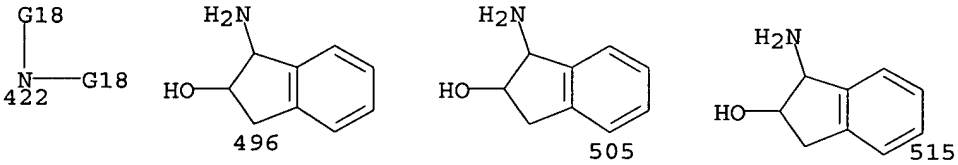


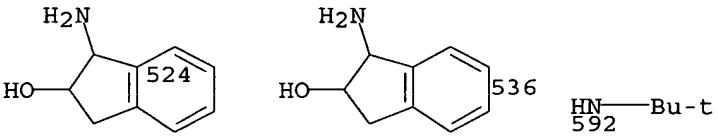




G16 = S(O) / SO2

G17 = R / 422 / aryl (opt. substd.) / carbocycle <containing 3 or more C> (opt. substd.) / heterocycle <containing 1-4 heteroatoms, zero or more N, zero or more S, zero or more O (no other heteroatoms)> (opt. substd.) / alkyl <containing 1-6 C> (opt. substd.) / alkenyl <containing 2-4 C> (opt. substd.) / cycloalkyl <containing 3-6 C> (opt. substd.) / cycloalkenyl <containing 5-6 C> (opt. substd.) / (Specifically claimed: 592 / 496 / 505 / 515 / 524 / 536)

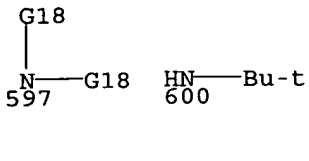


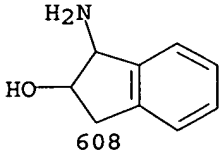


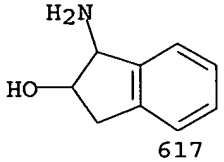
G18 = H / alkyl (opt. substd. by 1 or more G19) / alkenyl / alkynyl / aryl (opt. substd.) / carbocycle <containing 3 or more C> (opt. substd.) / heterocycle <containing 1-4 heteroatoms, zero or more N, zero or more S, zero or more O (no other heteroatoms)> (opt. substd.)

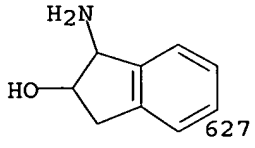
G19 = aryl (opt. substd.) / carbocycle <containing 3 or more C> (opt. substd.) / heterocycle <containing 1-4 heteroatoms, zero or more N, zero or more S,

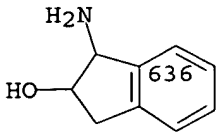
zero or more O (no other heteroatoms)> (opt. substd.)
G20 = **(1-2) CH2 (opt. substd.)**
G21 = alkyl <containing 1-6 C> (opt. substd.) /
alkenyl <containing 2-4 C> (opt. substd.)
G22 = R / 597 / aryl (opt. substd.) /
carbocycle <containing 3 or more C> (opt. substd.) /
heterocycle <containing 1-4 heteroatoms, zero or more N,
zero or more S, zero or more O (no other heteroatoms)>
(opt. substd.) / cycloalkyl <containing 3-6 C>
(opt. substd.) / cycloalkenyl <containing 5-6 C>
(opt. substd.) / (Specifically claimed: 600 / 608 / 617 /
627 / 636 / 648)

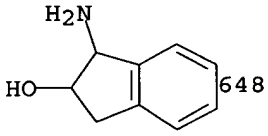








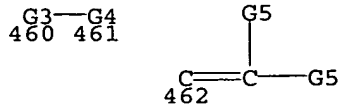




G27 = (1-2) C(O)
G37 = bond / NH (opt. substd.) / CH2 (opt. substd.)
G38 = 433 / 435 / 437

G16—G17 (433) G27—G21 (435) G27—G22 (437)

G44 = H / R
G45 = H / OH
G46 = H / OH
G47 = CH2 (opt. substd.) / CH2CH2 / NH (opt. substd.) /
460-446 461-449 / 462

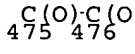


G48 = C(O) / SO2 / 466-445 467-448 / S(O)

C(O)-C(O)
466 467

G49 = **(1-3) CH2**
G50 = CH / **N**
G51 = NH (opt. substd.) / O / S / S(O) / SO2 / C(O) /
CH2 (opt. substd.)

G52 = C(O) / SO2 / **475-474 476-472** / S(O)



G53 = H / alkyl <containing 1-6 C> (opt. substd.) /
alkenyl <containing 2-6 C> (opt. substd.) /
alkynyl <containing 2-6 C> (opt. substd.) /
cycloalkyl <containing 3-6 C> (opt. substd.) /
cycloalkenyl <containing 5-6 C> (opt. substd.) / R
G55 = R / aryl (opt. substd.) /
carbocycle <containing 3 or more C> (opt. substd.) /
heterocycle <containing 1-4 heteroatoms, zero or more N,
zero or more S, zero or more O (no other heteroatoms)>
(opt. substd.) / **alkyl <containing 1-6 C> (opt. substd.)** /
alkenyl <containing 2-4 C> (opt. substd.) /
cycloalkyl <containing 3-6 C> (opt. substd.) /
cycloalkenyl <containing 5-6 C> (opt. substd.)
G58 = OMe / OH / NH2 / R
G6 +G7 = O
G45+G46= O
Patent location: claim 1
Note: substitution is restricted
Note: additional oxo formation and ring formation also claimed
Note: also incorporates broader disclosure

L41 ANSWER 26 OF 32 MARPAT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 129:246899 MARPAT
TITLE: Dryer-activated laundry additive compositions with color care agents and laundering colored fabrics
INVENTOR(S): Godfroid, Robert Allen; Wu, Ronghui; Littig, Janet Sue; Corona, Alessandro, III; Sivik, Mark Robert; Hartman, Fred Anthony; Honsa, Sandra Louise; Ditullio, Daniel Dale, Jr.
PATENT ASSIGNEE(S): The Procter & Gamble Co., USA
SOURCE: PCT Int. Appl., 32 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

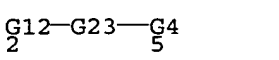
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9840459	A1	19980917	WO 1998-US2685	19980213
W: BR, CA, JP, MX				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2279857	AA	19980917	CA 1998-2279857	19980213
EP 970177	A1	20000112	EP 1998-906344	19980213
EP 970177	B1	20040421		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
BR 9807874	A	20000222	BR 1998-7874	19980213
JP 2001524141	T2	20011127	JP 1998-539565	19980213
AT 264904	E	20040515	AT 1998-906344	19980213
MX 9908011	A	20000131	MX 1999-8011	19990830
PRIORITY APPLN. INFO.:			US 1997-38904P	19970228

WO 1998-US2685 19980213

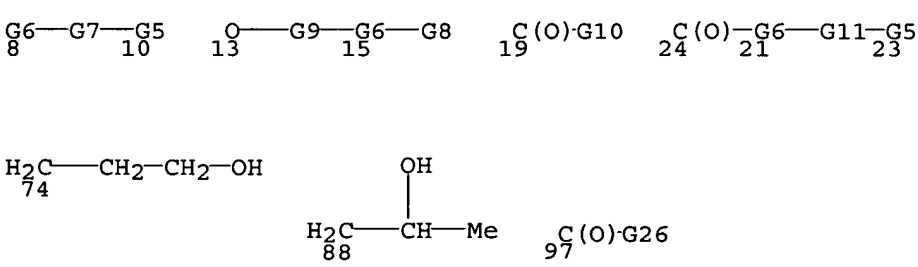
AB The dryer-activated laundry additive composition comprises .apprx.0.1-50% a color care agent R1R2NC(X2)nNR3R4 [X = H, alkyl; n = 0-6; R1-4 = H, (hydroxy)hydrocarbyl, alkoxy, carboxylic and phosphonic acids or their salts] and optional quaternary ammonium fabric softening compds., cyclodextrin, or a perfumes. Thus, a color care composition contained ditallow di-Me ammonium methylsulfate 58, N,N,N',N'-tetrakis-(2-hydroxypropyl)ethylenediamine 3, perfume 1, and stearic acid 38%.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

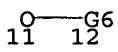
MSTR 1



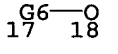
G1 = G3 / alkylene <containing 1-6 C> (substd. by 1 or more G2)
G2 = alkyl <containing 1-10 C> (opt. substd.) / aryl <containing 6 or more C> (opt. substd.)
G3 = (0-6) CH2
G4 = H / alkyl (opt. substd. by aryl) / aryl (opt. substd. by alkyl) / alkyl (substd. by 1 or more OH) / 8 / alkoxy / 13 / **alkyl <containing 1 or more C> (substd. by 97)** / PO3H2 (opt. substd. by alkyl) / 19 / 24 / (Specifically claimed: Et / Me / CH2CH2OH / 74 / 88)



G5 = OH / alkoxy <containing 1-10 C> (opt. substd.)
G6 = alkylene <containing 2-10 C, unbranched>
G7 = (0-9) 11-8 12-10

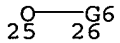


G8 = H / alkyl <containing 1-10 C> (opt. substd.)
G9 = (0-9) 17-13 18-15

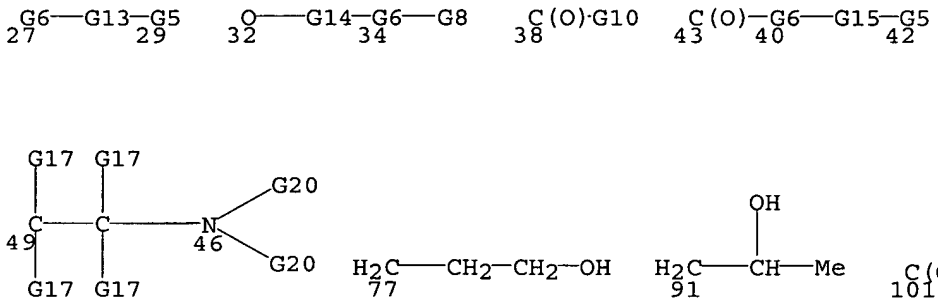


G10 = H / alkyl (opt. substd. by aryl) / aryl (substd. by alkyl) / alkyl (substd. by 1 or more OH) / OH / CO2H / **alkylcarbonyl (substd. by CO2H)** / PO3H2 (opt. substd. by alkyl)

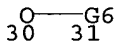
G11 = (0-9) 25-21 26-23



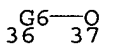
G12 = H / alkyl (opt. substd. by aryl) /
aryl (opt. substd. by alkyl) / alkyl (substd. by 1 or more OH) / 27 / alkoxy / 32 / alkyl <containing 1 or more C> (substd. by 101) / PO3H2 (opt. substd. by alkyl) / **38** / 43 / 49 / (Specifically claimed: Et / Me / CH2CH2OH / 77 / 91)



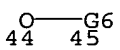
G13 = (0-9) 30-27 31-29



G14 = (0-9) 36-32 37-34

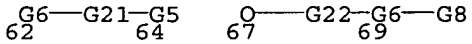


G15 = (0-9) 44-40 45-42

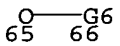


G17 = H / alkyl <containing 1-10 C> (opt. substd.) /
aryl <containing 6 or more C> (opt. substd.)

G20 = alkyl (opt. substd. by aryl) /
aryl (substd. by alkyl) / alkyl (substd. by 1 or more OH) / 62 / alkoxy / 67 / CO2H / alkylcarbonyl (substd. by CO2H) / PO3H2 (opt. substd. by alkyl)

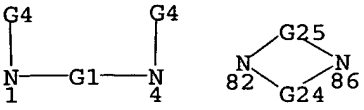


G21 = (0-9) 65-62 66-64

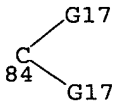


G22 = (0-9) 71-67 72-69

G23 = 1-2 4-5 / **82-2 86-5**



G24 = (0-6) 84



G25 = R <"moiety to complete a ring"> /
(Example: CH2CH2CH2CH2)
G26 = OH / 99

G27 = R <"salt-forming cation">
Derivative: and water soluble salts
Patent location: claim 1
Note: additional ring formation also disclosed

L41 ANSWER 27 OF 32 MARPAT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 129:230649 MARPAT
TITLE: Preparation of N-oxides of heterocyclic esters, amides, thioesters, and ketones as inhibitors of the enzyme activity associated with immunophilin proteins
INVENTOR(S): Hamilton, Gregory S.; Steiner, Joseph P.; Burak, Eric S.
PATENT ASSIGNEE(S): Guilford Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 67 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9837885	A1	19980903	WO 1998-US3484	19980226

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
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CA 2229707	AA	19980828	CA 1998-2229707	19980216	
ZA 9801474	A	19980608	ZA 1998-1474	19980223	
AU 9861815	A1	19980918	AU 1998-61815	19980226	
AU 723374	B2	20000824			
EP 993299	A1	20000419	EP 1998-906646	19980226	
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI					
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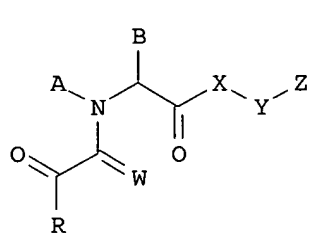
TW 458976	B	20011011	TW 1998-87102828	19980424	
US 6054452	A	20000425	US 1998-112319	19980709	
US 6251892	B1	20010626	US 2000-556482	20000421	
US 2001036942	A1	20011101	US 2001-842174	20010426	
US 6486151	B2	20021126			
PRIORITY APPLN. INFO.:			US 1997-807406	19970228	
			WO 1998-US3484	19980226	
			US 1998-112319	19980709	
			US 2000-556482	20000421	

GI



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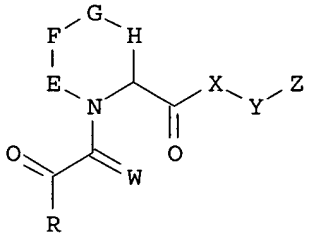

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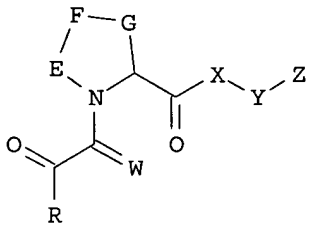
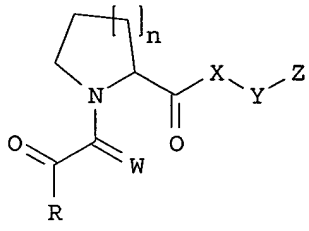


III



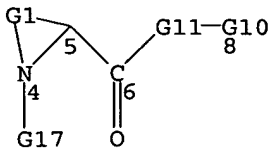
IV

AB The title compds. [I-IV; A and B, together with N and C atoms to which they are attached, = (un)saturated 5-7 membered heterocyclyl; E, F, G and H = CH2, O, S, etc.; W = O, S, CH2, H2; R = C1-6 alkyl, C1-6 alkenyl, etc.; X = O, NH, S, etc.; Y = a direct bond, C1-6 alkyl, C1-6 alkenyl, etc.; Z = an aromatic or tertiary alkyl amine oxidized to a corresponding N-oxide; n = 1-3], having an affinity for FKBP-type immunophilins, and therefore useful as inhibitors of the enzyme activity associated with immunophilin proteins, particularly peptidyl-prolyl isomerase, or rotamase activity, were prepared Thus, 5-step synthesis of (S)-IV [X = O; Y = (CH2)3; Z = 3-pyridyl

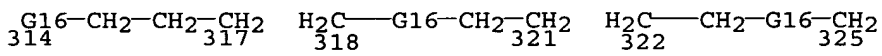
N-oxide; R = 1,1-dimethylpentyl; n = 1], which showed Ki of 225 nM against esterase degradation, is described.

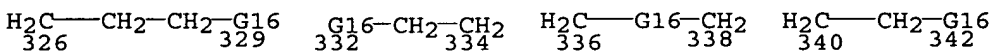
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

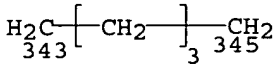
MSTR 1



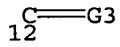
G1 = R <"moiety necessary to complete a 5- to 7-membered ring"> / (Specifically claimed: CH2CH2CH2CH2 / 314-4 317-5 / 318-4 321-5 / 322-4 325-5 / 326-4 329-5 / CH2CH2CH2 / **332-4 334-5** / 336-4 338-5 / 340-4 342-5)





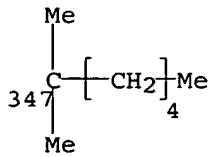


G2 = **12** / C=CH2 / CH2



G3 = **O** / S

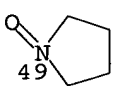
G4 = **alkyl <containing 1-6 C> (opt. substd. by 1 or more G5)** / alkenyl <containing 2-6 C> (opt. substd. by 1 or more G5) / (Example: 347)

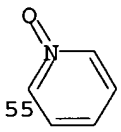


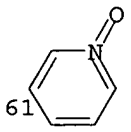
G5 = (1) G6 / alkyl <containing 1-4 C> / alkenyl <containing 2-4 C> / OH

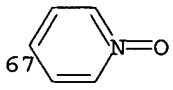
G6 = cycloalkyl <containing 3-8 C> (opt. substd. by 1 or more G7)

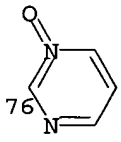
G7 = alkyl <containing 1-4 C> /
alkenyl <containing 2-4 C> / OH
G8 = H / F / Cl / Br / I / OH / NO2 / CF3 /
alkyl <containing 1-6 C> / alkenyl <containing 2-6 C> /
alkenyloxy <containing 2-4 C> / OPh / OCH2Ph / NH2
G9 = F / Cl / Br / I / OH / NO2 / CF3 /
alkyl <containing 1-6 C> / alkenyl <containing 2-6 C> /
alkenyloxy <containing 2-4 C> / OPh / OCH2Ph / NH2
G10 = 49 / 55 / 61 / 67 / 76 / 83 / 90 / 97 / 104 / 111 /
118 / 125 / 132 / 139 / 144 / 156 / 168 / 183 / 195 / 207 /
219 / 226 / 233 / 245 / 260 / 272 / 284 / 296 / 299

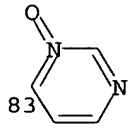


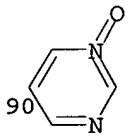


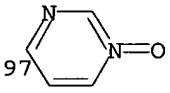


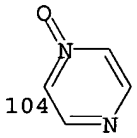


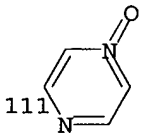


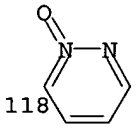


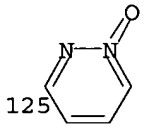


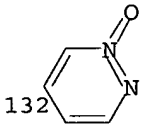


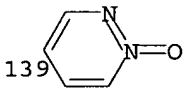


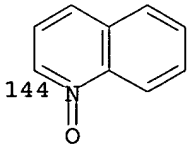


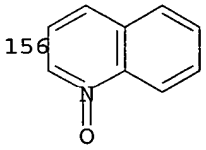


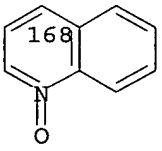


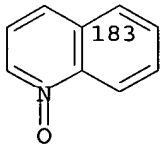


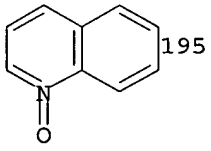


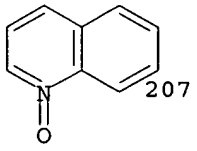


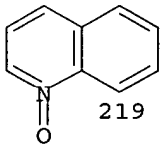


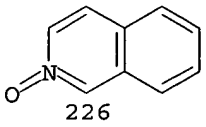


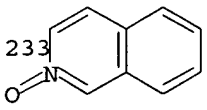


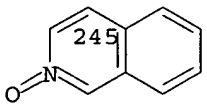


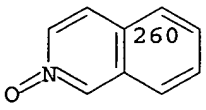


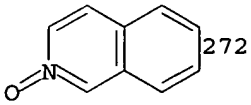


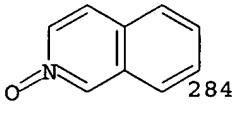


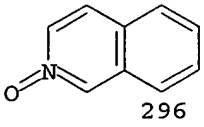


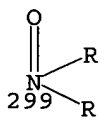




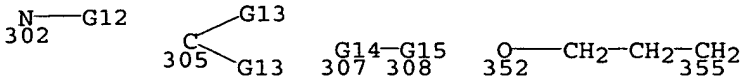




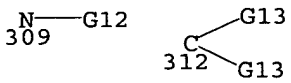




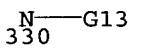
G11 = O / NH / 302 / S / 305 / 307-6 308-8 /
(Example: 352-6 355-8)



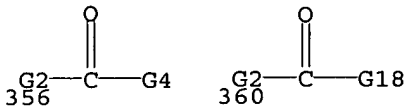
G12 = alkyl <containing 1-4 C> /
alkenyl <containing 3-4 C> / alkynyl <containing 3-4 C> / R
G13 = H / **alkyl <containing 1-4 C>** /
alkenyl <containing 3-4 C> / alkynyl <containing 3-4 C> / R
G14 = O / NH / 309 / S / 312



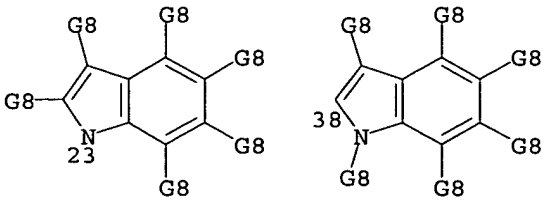
G15 = alkylene <containing 1-6 C> (opt. substd.) /
alkenylene <containing 2-6 C> (opt. substd.)
G16 = O / S / S(O) / SO2 / **330**



G17 = **356** / 360



G18 = cycloalkyl <containing 3-5 C>
(opt. substd. by 1 or more G7) /
cycloalkenyl <containing 5-7 C>
(opt. substd. by 1 or more G7) /
naphthyl (opt. substd. by 1 or more G9) / 23 / 38 /
furyl (opt. substd. by 1 or more G9) /
thienyl (opt. substd. by 1 or more G9) /
pyridyl (opt. substd. by 1 or more G9) /
Ph (opt. substd. by 1 or more G9)



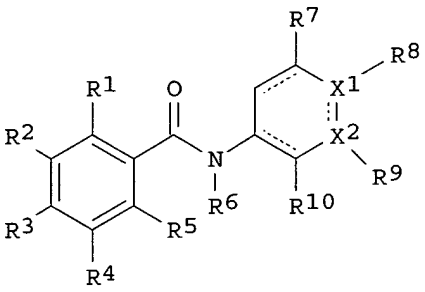
Derivative: or pharmaceutically acceptable salts
Patent location: claim 1

L41 ANSWER 28 OF 32 MARPAT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 129:310895 MARPAT
TITLE: Benzamide compounds and their use as neovascularization inhibitors
INVENTOR(S): Inaba, Takayuki; Tada, Hiroki; Iwamura, Hiroyuki
PATENT ASSIGNEE(S): Japan Tobacco, Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 106 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10259176	A2	19980929	JP 1997-84463	19970317

PRIORITY APPLN. INFO.: JP 1997-84463 19970317
GI



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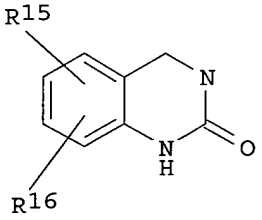
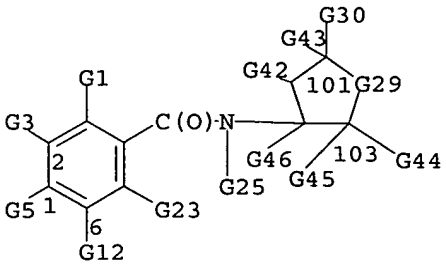


II

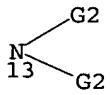
AB The inhibitors contain benzamides I [R1 = H, NO2, halo, cyano, lower alkoxy, NR11R12 (R11, R12 = H, acyl); R2 = H, NO2, halo, OR13 (R13 = lower alkyl, aralkyl, cycloalkyl); R3 = X3(CH2)mR14 [R14 = (un)substituted Ph, (un)substituted heteroaryl, (un)substituted amino, (un)substituted lower alkyl, cycloalkyl, acyl, alkenyl, H; X3 = O, NHCO, OSO2, NR17 (R17 = H, lower alkyl); m = 0-5], II (R15, R16 = H, lower alkoxy, amino, lower alkyl, CO2H, OH); R2 and R3 may be bonded to form a condensed 1,3-oxazole ring; R4 = H, OR19 (R19 = lower alkyl, aralkyl, cycloalkyl); R3 and R4 may be bonded to form a condensed 1,3-oxazole, 1,4-oxazine, or pyrimidine ring; R5 = H, NO2, alkenyl; NHR28 (R28 = H, acyl, lower alkoxycarbonyl); R6 = H, (un)substituted lower alkyl; R5 and R6 may be bonded to form a condensed pyrimidine, diazepine, or pyridine ring; R7 = H, lower alkoxy; R8 = X4(CH2)tR30 [X4 = O, CH2, CO, CONH, OSO2, SO2NH, NR31 (R31 = H, lower alkyl, aralkyl), direct bond], t = 0-5; R30 = (un)substituted Ph, (un)substituted heteroaryl, (un)substituted amino, H, OH, halo, lower alkyl, lower alkoxy, cycloalkyl, acyl, cyano, CO2R32 (R32 = H, lower

alkyl); R9 = H, lower alkoxycarbonyl, halo, OR33 (R33 = H, lower alkyl, aralkyl), CONHR34 (R34 = H, lower alkyl, aralkyl); R7 and R8, R8 and R9 may be bonded to form a 1,3-oxazole ring; X1, X2 =X, N; dotted line represents an optional double bond]. I are useful for treatment of rheumatoid arthritis, diabetic retinopathy, neoplasms, etc. IC50 of 4-benzyloxy-N-(4-benzyloxyphenyl)-3-methoxybenzamide (preparation given) against bFGF- or VEGF-induced proliferation of HUVEC was 0.85 μM.

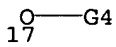
MSTR 1A



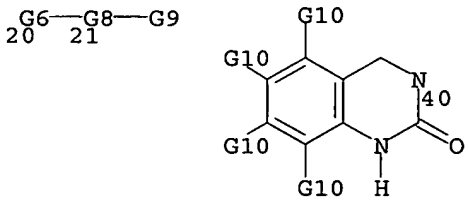
G1 = H / NO2 / F / Cl / Br / I / CN / alkoxy <containing 1-6 C> / 13



G2 = H / acyl
G3 = H / NO2 / F / Cl / Br / I / 17



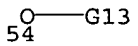
G4 = alkyl <containing 1-6 C> (opt. substd. by 1 or more aryl) / cycloalkyl <containing 3-10 C>
G5 = 20 / 40



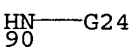
G6 = O / 23-1 24-21 / 27-1 28-21 / 31

G7 = H / alkyl <containing 1-6 C>
G8 = (0-5) CH2

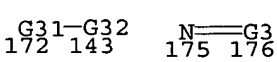
G9 = Ph (opt. substd.) / heteroaryl (opt. substd.) / NH2 (opt. substd.) / alkyl <containing 1-6 C> (opt. substd.) / cycloalkyl <containing 3-10 C> / acyl / alkenyl / H
G10 = 2 or more H / alkoxy <containing 1-6 C> / NH2 / alkyl <containing 1-6 C> / CO2H / OH
G11 = Ph (opt. substd.) / heteroaryl (opt. substd.) / alkyl <containing 1-6 C> (opt. substd. by 1 or more aryl (opt. substd.)) / alkoxy <containing 1-6 C> / NH2 (opt. substd.) / OH / NO2 / CHO / H
G12 = H / 54



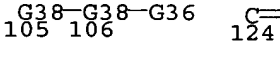
G13 = alkyl <containing 1-6 C> (opt. substd. by 1 or more aryl) / cycloalkyl <containing 3-10 C>
G15 = (0-5) CH2
G16 = Ph (opt. substd.) / heteroaryl (opt. substd.) / NH2 (opt. substd.) / CO2H / alkoxycarbonyl <containing 1-6 C> / OH / H
G17 = CH2 / C(O)
G18 = (0-1) CH2
G19 = 2 or more H / alkyl <containing 1-6 C> / alkoxy <containing 1-6 C>
G20 = (0-5) CH2
G21 = aryl (opt. substd.) / heteroaryl (opt. substd.)
G22 = H / alkyl <containing 1-6 C>
G23 = H / NO2 / alkenyl / 90



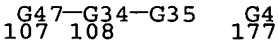
G24 = H / acyl / alkoxycarbonyl <containing 1-6 C>
G25 = H / alkyl <containing 1-6 C> (opt. substd.)
G29 = 172 / 175-101 176-103



G30 = H / alkoxy <containing 1-6 C>
G31 = 105-101 106-103 105-143 / 124-101 125-103 124-143



G32 = Ph (opt. substd.) / heteroaryl (opt. substd.) / NH2 (opt. substd.) / H / OH / F / Cl / Br / I / alkyl <containing 1-6 C> / alkoxy <containing 1-6 C> / cycloalkyl <containing 3-10 C> / 179 / CN / 177 / 107 / 183



G33 = H / alkyl <containing 1-6 C>
(opt. substd. by 1 or more aryl)
G34 = alkylene <containing 1-5 C, unbranched>
G35 = alkyl <containing 1-6 C> / **181** / CN

C(O)-G40
181

G36 = H / **alkoxycarbonyl <containing 1-6 C>** / F / Cl /
Br / I / OH / alkoxy <containing 1-6 C>
(opt. substd. by 1 or more aryl) / 121

C(O)-NH—G37
121

G37 = H / alkyl <containing 1-6 C>
(opt. substd. by 1 or more aryl)
G38 = CH / **N**
G39 = N / 173

C——G36
173

G40 = H / R / OH / alkoxy <containing 1-6 C>
G41 = Ph (opt. substd.) / heteroaryl (opt. substd.) /
NH2 (opt. substd.) / H / OH / F / Cl / Br / I /
alkoxy <containing 1-6 C> / cycloalkyl <containing 3-10 C>
G42 = H
G43 = H
G44 = H / OH / alkoxy <containing 1-6 C>
(opt. substd. by 1 or more aryl) / OPh
G45 = H
G46 = H
G47 = O / CH2 / C(O) / 110-172 111-108 /
114-172 115-108 / 118 / CH=CH

G52—NH O——SO2 N——G33
110 111 114 115 118

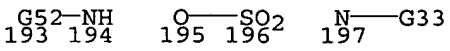
G48 = O / **C(O)** / 146-172 147-178 / 150-172 151-178 /
156 / CH=CH / alkylene

G52—NH O——SO2 N——G33
146 147 150 151 156

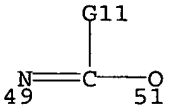
G49 = O / C(O) / 185-172 186-184 / 187-172 188-184 /
189 / CH=CH / alkylene / 191-172 192-184

G52—NH O——SO2 N——G33 G50—G34
185 186 187 188 189 191 192

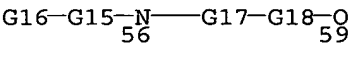
G50 = O / CH2 / C(O) / 193-172 194-192 /
195-172 196-192 / 197 / CH=CH

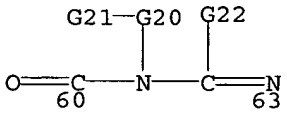


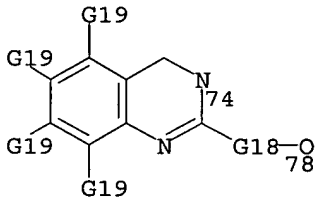
G52 = C(O) / SO2
G3 +G5 = 49-2 51-1



G5 +G12= 56-1 59-6 / 74-1 78-6 / 60-1 63-6

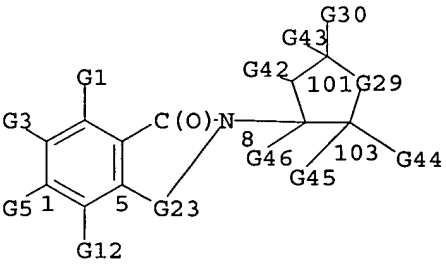




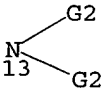


G42+G43= bond
G45+G46= bond
Derivative: or pharmaceutically acceptable salts
Patent location: claim 1
Note: additional ring formation also claimed

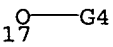
MSTR 1B



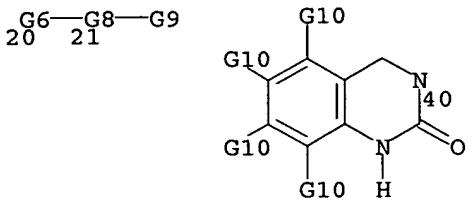
G1 = H / NO2 / F / Cl / Br / I / CN /
alkoxy <containing 1-6 C> / 13



G2 = H / acyl
G3 = H / NO2 / F / Cl / Br / I / 17



G4 = alkyl <containing 1-6 C>
(opt. substd. by 1 or more aryl) /
cycloalkyl <containing 3-10 C>
G5 = 20 / 40



G6 = O / 23-1 24-21 / 27-1 28-21 / 31

HN—C(O) O—SO2 N—G7
23 24 27 28 31

G7 = H / alkyl <containing 1-6 C>
G8 = (0-5) CH2
G9 = Ph (opt. substd.) / heteroaryl (opt. substd.) /
NH2 (opt. substd.) / alkyl <containing 1-6 C>
(opt. substd.) / cycloalkyl <containing 3-10 C> / acyl /
alkenyl / H
G10 = 2 or more H / alkoxy <containing 1-6 C> / NH2 /
alkyl <containing 1-6 C> / CO2H / OH
G12 = H / 54

O—G13
54

G13 = alkyl <containing 1-6 C>
(opt. substd. by 1 or more aryl) /
cycloalkyl <containing 3-10 C>
G23 = 93-5 95-8 / 96-5 97-8

HN—C(O)-G26 G27=C—G28
93 95 96 97

G26 = (0-1) CH2
G27 = N / CH
G28 = H / alkyl <containing 1-6 C>
G29 = 172 / 175-101 176-103

G31—G32 N=G39
172 143 175 176

G30 = H / alkoxy <containing 1-6 C>
G31 = 105-101 106-103 105-143 / 124-101 125-103 124-143

G38—G38—G36 C=G39
105 106 124 125

G32 = Ph (opt. substd.) / heteroaryl (opt. substd.) /
NH2 (opt. substd.) / H / OH / F / Cl / Br / I /
alkyl <containing 1-6 C> / alkoxy <containing 1-6 C> /
cycloalkyl <containing 3-10 C> / 179 / CN / 177 / 107 / 183

G47—G34—G35 G48—G35 C(O)-G40 G49—G41
107 108 177 178 179 183 184

G33 = H / alkyl <containing 1-6 C>
(opt. substd. by 1 or more aryl)
G34 = alkylene <containing 1-5 C, unbranched>
G35 = alkyl <containing 1-6 C> / **181** / CN

C(O)-G40
181

G36 = H / **alkoxycarbonyl <containing 1-6 C>** / F / Cl /
Br / I / OH / alkoxy <containing 1-6 C>
(opt. substd. by 1 or more aryl) / 121

C(O)-NH—G37
121

G37 = H / alkyl <containing 1-6 C>
(opt. substd. by 1 or more aryl)
G38 = CH / **N**
G39 = N / 173

C——G36
173

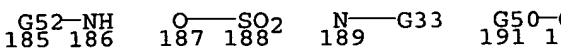
G40 = H / R / OH / alkoxy <containing 1-6 C>
G41 = Ph (opt. substd.) / heteroaryl (opt. substd.) /
NH2 (opt. substd.) / H / OH / F / Cl / Br / I /
alkoxy <containing 1-6 C> / cycloalkyl <containing 3-10 C>
G42 = H
G43 = H
G44 = H / OH / alkoxy <containing 1-6 C>
(opt. substd. by 1 or more aryl) / OPh
G45 = H
G46 = H
G47 = O / CH2 / C(O) / 110-172 111-108 /
114-172 115-108 / 118 / CH=CH

G52—NH O——SO2 N——G33
110 111 114 115 118

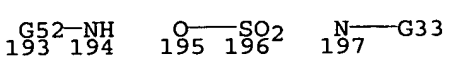
G48 = O / **C(O)** / 146-172 147 178 / 150-172 151-178 /
156 / CH=CH / alkylene

G52—NH O——SO2 N——G33
146 147 150 151 156

G49 = O / C(O) / 185-172 186-184 / 187-172 188-184 / 189 / CH=CH / alkylene / 191-172 192-184



G50 = O / CH2 / C(O) / 193-172 194-192 / 195-172 196-192 / 197 / CH=CH



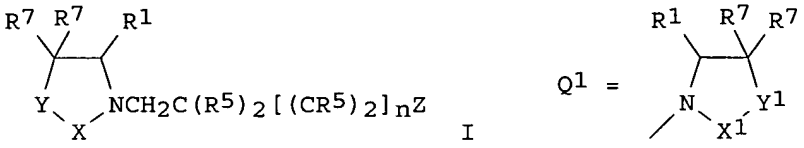
G52 = C(O) / SO2
G42+G43= bond
G45+G46= bond
Derivative: or pharmaceutically acceptable salts
Patent location: claim 1
Note: additional ring formation also claimed

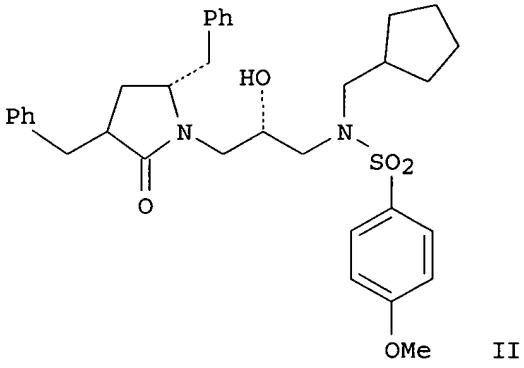
L41 ANSWER 29 OF 32 MARPAT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 130:209597 MARPAT
Correction of: 127:205470
TITLE: Preparation of heterocyclylhydroxyalkanamides and related compounds as HIV protease inhibitors.
INVENTOR(S): Tung, Roger Dennis; Salituro, Francesco Gerald; Deininger, David D.; Bhisetti, Govinda Rao; Baker, Christopher Todd; Spaltenstein, Andrew; Kazmierski, Wieslaw M.; Andrews, Clarence Webster III
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 336 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9727180	A1	19970731	WO 1997-US1610	19970122
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5883252	A	19990316	US 1996-592777	19960126
US 5945413	A	19990831	US 1996-724563	19960930
AU 9717580	A1	19970820	AU 1997-17580	19970122
AU 709239	B2	19990826		
EP 882022	A1	19981209	EP 1997-904911	19970122
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9707086	A	19990413	BR 1997-7086	19970122
JP 2000501111	T2	20000202	JP 1997-527124	19970122

NO 9803435 A 19980921 NO 1998-3435 19980724
PRIORITY APPLN. INFO.: US 1996-592777 19960126
US 1996-724563 19960930
WO 1997-US1610 19970122

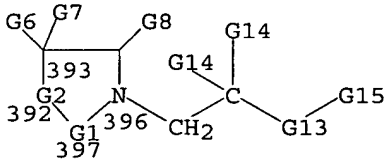
GI





AB Title compds. [I; Z = (QR1)R1R4, Q1, etc.; ; X, X1 = CO, CO2, SO, SO2; Y, Y1 = [C(R2)2]p, NR2, C:C(R2)2, NR2CH2, etc.; Q = CH, N; R1, R2 = H, (substituted) alkyl, alkenyl, alkynyl, (fused) cycloalkyl, cycloalkenyl, etc.; R4 = (substituted) OR9, XR9, N(R9)2, R6, alkyl, alkenyl, (fused) cycloalkyl, cycloalkenyl, etc.; R5 = H, OH, O, R1; R6 = (substituted) aryl, carbocyclyl, heterocyclyl; R7 = H, OH, O; R9 = H, alkyl, alkenyl, alkynyl, aryl, carbocyclyl, heterocyclyl, aralkyl, carbocyclylalkyl, heterocyclylalkyl; n = 1, 2; r = 0-2], were prepared Thus, title compound (II) (preparation given) inhibited HIV protease with Ki = 1.5 nM.

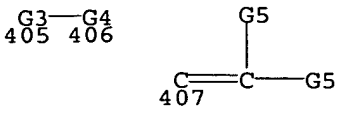
MSTR 1A



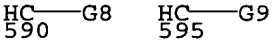
G1 = C(O) / SO2 / 13-392 14-396 / S(O)

C(O)-C(O)
13 14

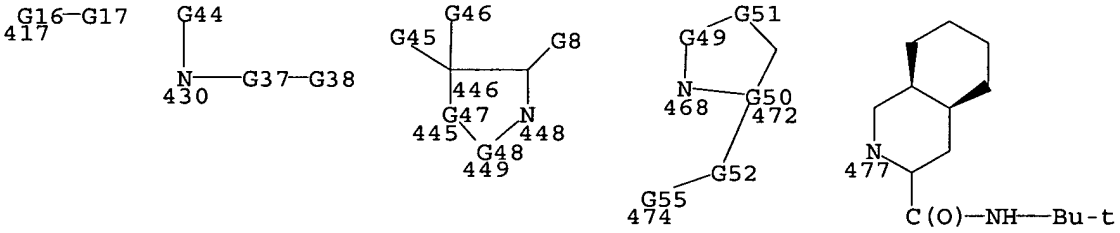
G2 = CH2 (opt. substd.) / CH2CH2 / NH (opt. substd.) / 405-393 406-397 / 407

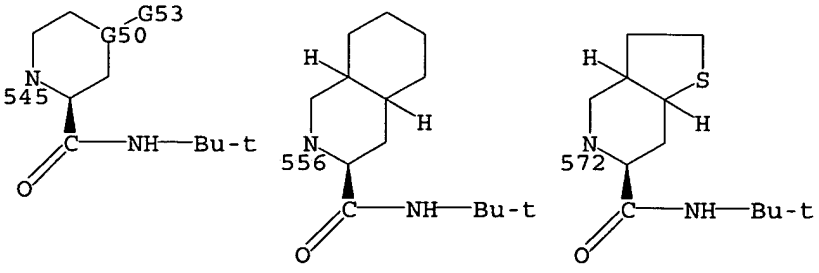


G3 = NH (opt. substd.) / O / S / S(O) / SO2
G4 = (1-2) CH2
G5 = H / R
G6 = H / OH
G7 = H / OH
G8 = H / aryl (opt. substd.) / carbocycle <containing 3 or more C> (opt. substd.) / heterocycle <containing 1-4 heteroatoms, zero or more N, zero or more S, zero or more O (no other heteroatoms)> (opt. substd.) / cycloalkyl <containing 3-6 C> (opt. substd.) / cycloalkenyl <containing 5-6 C> (opt. substd.)
G9 = carbon chain <containing 1-6 C, 0 or more double bonds, 0 or more triple bonds> (opt. substd.) / (Specifically claimed: CH2Ph (opt. substd. by G58))
G13 = G20 / (Specifically claimed: 590 / 595 / C(O))



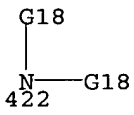
G14 = H / OH / R
G15 = 417 / 430 / 448 / **468** / (Specifically claimed: 477 / 545 / 556 / 572)

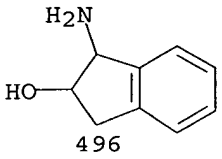


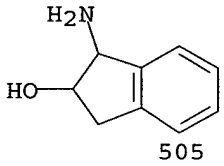


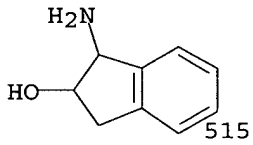
G16 = S / S(O) / SO2

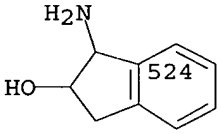
G17 = R / 422 / aryl (opt. substd.) / carbocycle <containing 3 or more C> (opt. substd.) / heterocycle <containing 1-4 heteroatoms, zero or more N, zero or more S, zero or more O (no other heteroatoms)> (opt. substd.) / alkyl <containing 1-6 C> (opt. substd.) / alkenyl <containing 2-4 C> (opt. substd.) / cycloalkyl <containing 3-6 C> (opt. substd.) / cycloalkenyl <containing 5-6 C> (opt. substd.) / (Specifically claimed: 592 / 496 / 505 / 515 / 524 / 536)

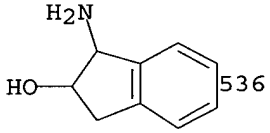


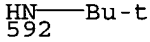












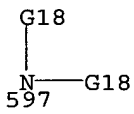
G18 = H / alkyl (opt. substd. by 1 or more G19) / alkenyl / alkynyl / aryl (opt. substd.) / carbocycle <containing 3 or more C> (opt. substd.) / heterocycle <containing 1-4 heteroatoms, zero or more N, zero or more S, zero or more O (no other heteroatoms)> (opt. substd.)

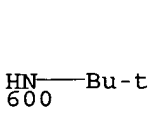
G19 = aryl (opt. substd.) / carbocycle <containing 3 or more C> (opt. substd.) / heterocycle <containing 1-4 heteroatoms, zero or more N, zero or more S, zero or more O (no other heteroatoms)> (opt. substd.)

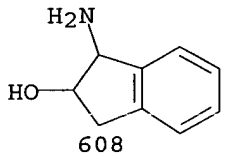
G20 = **(1-2) CH2 (opt. substd.)**

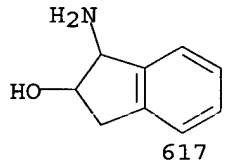
G21 = alkyl <containing 1-6 C> (opt. substd.) / alkenyl <containing 2-4 C> (opt. substd.)

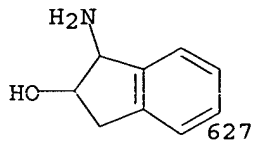
G22 = R / 597 / aryl (opt. substd.) / carbocycle <containing 3 or more C> (opt. substd.) / heterocycle <containing 1-4 heteroatoms, zero or more N, zero or more S, zero or more O (no other heteroatoms)> (opt. substd.) / cycloalkyl <containing 3-6 C> (opt. substd.) / cycloalkenyl <containing 5-6 C> (opt. substd.) / (Specifically claimed: 600 / 608 / 617 / 627 / 636 / 648)

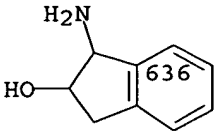


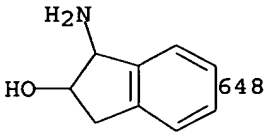










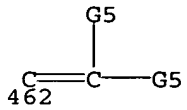


G27 = (1-2) C(O)
G37 = bond / NH (opt. substd.) / CH2 (opt. substd.)
G38 = 433 / 435 / 437

G16—G17 G27—G21 G27—G22
433 435 437

G44 = H / R
G45 = H / OH
G46 = H / OH
G47 = CH2 / CH2CH2 / NH (opt. substd.) /
460-446 461-449 / 462

G3—G4
460 461



G48 = C(O) / SO2 / 466-445 467-448 / S(O)

C(O)-C(O)
466 467

G49 = **(1-3) CH2**
G50 = CH / **N**
G51 = NH (opt. substd.) / O / S / S(O) / SO2 / C(O) /
CH2 (opt. substd.)
G52 = C(O) / SO2 / **475-474 476-472** / S(O)

C(O)-C(O)
475 476

G53 = H / alkyl <containing 1-6 C> (opt. substd.) /
alkenyl <containing 2-6 C> (opt. substd.) /
alkynyl <containing 2-6 C> (opt. substd.) /
cycloalkyl <containing 3-6 C> (opt. substd.) /
cycloalkenyl <containing 5-6 C> (opt. substd.) / R
G55 = R / aryl (opt. substd.) /
carbocycle <containing 3 or more C> (opt. substd.) /
heterocycle <containing 1-4 heteroatoms, zero or more N,
zero or more S, zero or more O (no other heteroatoms)>
(opt. substd.) / **alkyl <containing 1-6 C> (opt. substd.)** /
alkenyl <containing 2-4 C> (opt. substd.) /
cycloalkyl <containing 3-6 C> (opt. substd.) /
cycloalkenyl <containing 5-6 C> (opt. substd.)
G58 = OMe / OH / NH2 / R
G6 +G7 = O
G45+G46= O

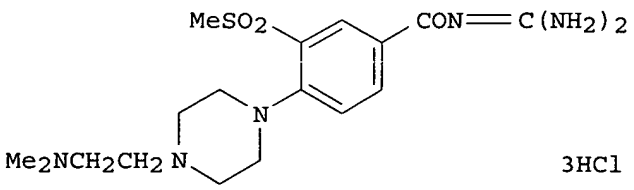
Patent location: claim 1
Note: substitution is restricted
Note: additional oxo formation and ring formation also claimed

L41 ANSWER 30 OF 32 MARPAT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 127:149157 MARPAT
TITLE: Preparation of benzoylguanidines as cell proliferation inhibitors
INVENTOR(S): Buerger, Erich; Eickmeier, Christian; Roos, Otto
PATENT ASSIGNEE(S): Boehringer Ingelheim Kg, Germany
SOURCE: Ger. Offen., 15 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19601303	A1	19970717	DE 1996-19601303	19960116
ZA 9700277	A	19970716	ZA 1997-277	19970114
TW 426673	B	20010321	TW 1997-86100385	19970115
CA 2240075	AA	19970724	CA 1997-2240075	19970116
WO 9726253	A1	19970724	WO 1997-EP177	19970116
W: AU, BG, BR, BY, CA, CN, CZ, EE, HU, IL, JP, KR, KZ, LT, LV, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9714429	A1	19970811	AU 1997-14429	19970116
AU 722619	B2	20000810		
EP 882031	A1	19981209	EP 1997-901043	19970116
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
CN 1208409	A	19990217	CN 1997-191727	19970116
CN 1072663	B	20011010		
BR 9707002	A	19990720	BR 1997-7002	19970116
JP 2000503309	T2	20000321	JP 1997-525687	19970116
NZ 326347	A	20010330	NZ 1997-326347	19970116
RU 2181720	C2	20020427	RU 1998-115533	19970116
SK 282751	B6	20021203	SK 1998-957	19970116
NO 9803261	A	19980715	NO 1998-3261	19980715
NO 311517	B1	20011203		
US 6114335	A	20000905	US 1998-101792	19980925
HK 1016981	A1	20020308	HK 1999-102143	19990513

PRIORITY APPLN. INFO.: DE 1996-19601303 19960116
WO 1997-EP177 19970116

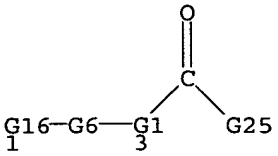
GI



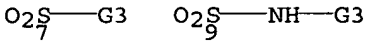
I

AB RCONHC(:NH)NH2 [R = substituted Ph] were prepared fo use as inhibitors of cell proliferation. Thus, the guanidine I was obtained by treating the acid with guanidine hydrochloride. I had an IC50 for inhibition of the Na+/H+ exchanger of 0.500 mM.

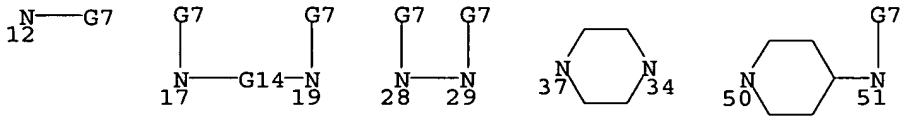
MSTR 1A

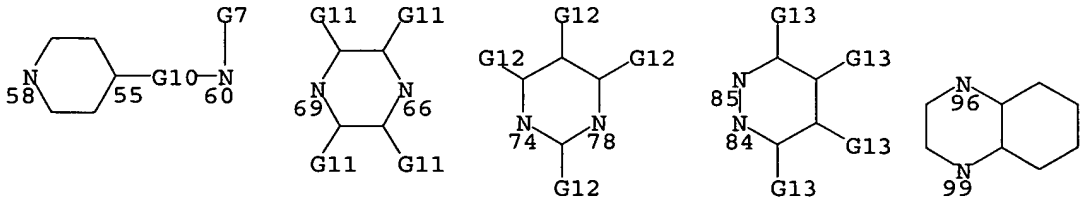


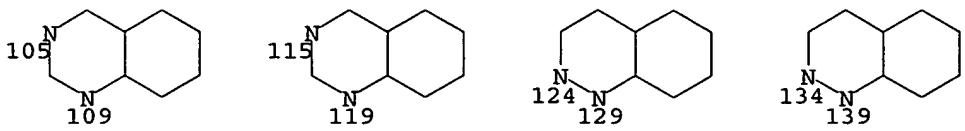
G1 = **phenylene (substd. by (1) G2)**
G2 = 7 / 9 / F / Cl / CF3

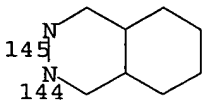


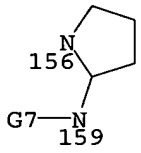
G3 = alkyl <containing 1-8 C>
(opt. substd. by 1 or more G4) / (Example: Me)
G4 = F / Cl / Br / I / Ph (opt. substd.) /
carbocycle <containing 6 C, aromatic, bonds all normalized, 6-membered monocyclic ring> (substd. by (1-3) G5)
G5 = F / Cl / Br / I / alkyl <containing 1-4 C> /
alkoxy <containing 1-4 C>
G6 = 12 / 17-1 19-3 / 28-1 29-3 / 37-1 34-3 /
50-1 51-3 / 58-1 60-3 / 69-1 66-3 / 74-1 78-3 /
85-1 84-3 / 96-1 99-3 / 105-1 109-3 / 119-1 115-3 /
124-1 129-3 / 139-1 134-3 / 144-1 145-3 / 156-1 159-3 /
162-1 165-3 / 174-1 176-3 / 177-1 186-3

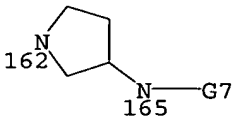


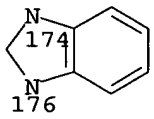


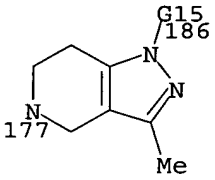




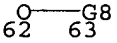




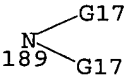


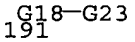


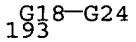
G7 = H / alkyl <containing 1-4 C> / Ph / CH2Ph / cycloalkyl <containing 3-7 C>
G8 = alkylene <containing 1-6 C>
G10 = O / alkylene <containing 1-6 C> / 62-55 63-60

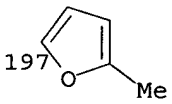


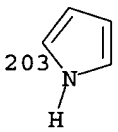
G11 = 2 or more H / alkyl <containing 1-4 C> / Ph / CH2Ph / cycloalkyl <containing 3-7 C>
G12 = 2 or more H / alkyl <containing 1-4 C> / Ph / CH2Ph / cycloalkyl <containing 3-7 C>
G13 = 2 or more H / alkyl <containing 1-4 C> / Ph / CH2Ph / cycloalkyl <containing 3-7 C>
G14 = alkylene <containing 1-6 C> / cyclohexylene
G15 = NH (opt. substd.)
G16 = alkyl <containing 1-8 C> (opt. substd.) / aryl (opt. substd.) / 189 / heterocycle <containing zero or more N, zero or more O, zero or more S (no other heteroatoms), mono- or bicyclic, (up to 1) 5-membered, (up to 2) 6-membered rings only> (opt. substd.) / 191 / 193 / (Examples: 2-furyl / 2-thienyl / 197 / Ph / 203)





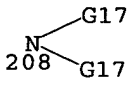






G17 = H / alkyl <containing 1-8 C> / aryl / aralkyl
G18 = G19 / G20 / G21 / G22 / NH (opt. substd.)
G19 = (1-8) CH2
G20 = (1-2) CHOH
G21 = **(1-2) C(O)**
G22 = (1-2) C(S)
G23 = **alkyl <containing 1-8 C> (opt. substd.)**
G24 = aryl (opt. substd.) / 208 / heterocycle <containing zero or more N, zero or more O, zero or more S (no other heteroatoms), mono- or bicyclic,

(up to 1) 5-membered, (up to 2) 6-membered rings only>
(opt. substd.)

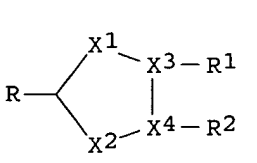


G25 = NHC(NH)NH2 / OH
Patent location: claim 1
Note: also incorporates structure IV in claim 4

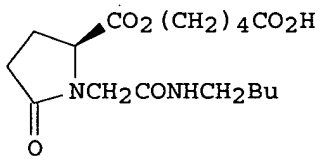
L41 ANSWER 31 OF 32 MARPAT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 120:270095 MARPAT
TITLE: Preparation of heteroprostanoids as drugs
INVENTOR(S): Casini, Giovanni
PATENT ASSIGNEE(S): Nuovo Consorzio Sanitario Nazionale, Italy
SOURCE: Eur. Pat. Appl., 19 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 572365	A2	19931201	EP 1993-830237	19930528
EP 572365	A3	19940427		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
PRIORITY APPLN. INFO.: IT 1992-RM412 19920529
GI



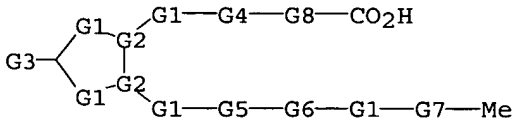
I



II

AB Title compds. [I; R = H or OH; R1 = Z1Z3(CH2)nCO2H; R2 = Z2Z4Z5Z6(CH2)mMe; X1,X2,Z1,Z2,Z6 = CH2 or CO; X3,X4 = N or CH; Z3 = CH2, NH, O; Z4 = NH, CH2, CO; Z5 = CH2 or NH; m = 0-4; n = 0-5] were prepared as, e.g., thrombocyte aggregation inhibitors. Thus, L-pyroglutamic acid was esterified by Br(CH2)4CO2CH2Ph and the product N-alkylated by ICH2CON(CH2Ph)CH2Bu (preparation given) to give, after deprotection, title compound II which had EC50 5x10-6M for thrombocyte aggregation inhibition in vitro.

MSTR 1

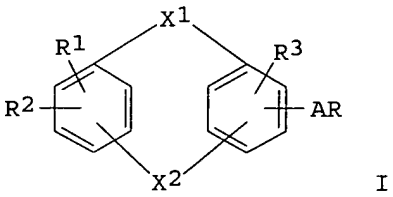


G1 = **CH2** / **C(O)**
G2 = **N** / CH
G3 = H / OH
G4 = CH2 / NH / O
G5 = NH / CH2 / **C(O)**
G6 = **CH2** / NH
G7 = (0-4) CH2
G8 = (0-5) CH2
Derivative: and pharmaceutically tolerable salts
Patent location: claim 1

L41 ANSWER 32 OF 32 MARPAT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 116:41309 MARPAT
TITLE: Preparation of (heterocyclylalkyl)paracyclophanes and analogs as cardiovascular agents
INVENTOR(S): Psiorz, Manfred; Trach, Volker
PATENT ASSIGNEE(S): Thomae, Dr. Karl, G.m.b.H., Germany
SOURCE: Eur. Pat. Appl., 38 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 450429	A1	19911009	EP 1991-104535	19910322
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
DE 4010531	A1	19911010	DE 1990-4010531	19900402
CA 2039466	AA	19911003	CA 1991-2039466	19910328
US 5147882	A	19920915	US 1991-678556	19910328
JP 04221349	A2	19920811	JP 1991-68437	19910401

PRIORITY APPLN. INFO.: DE 1990-4010531 19900402
GI

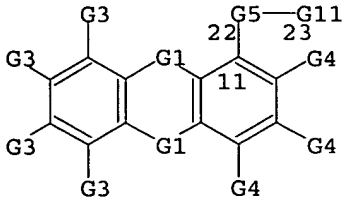


I

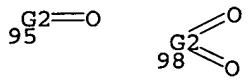
AB The title compds. [I; A = alkylene, Y1A1, Y2A2; A1,A2 = alkylene; R = cyano, NR5R6, C(:NR7)NHR8; R1-R4 = H, halo, OH, alkyl, alkoxy, alkylsulfonyloxy; R5 = H, (cyclo)alkyl, phenylalkyl, etc.; R6-R8 = H, alkyl; NR5R6 = heterocyclyl; X1, X2 = alkylene, alkenylene; Y1 = O, SOn; Y2 = CH:CH, C.tplbond.C; n = 0-2] were prepared Thus, 4-(3-bromopropyl)[2.2]paracyclophane was condensed with N,N-dimethyl-3-(3-

piperidyl)propionamide to give 4-[3-[3-(3-dimethylamino-3-oxopropyl)-1-piperidyl]propyl][2.2]paracyclophane which gave 48.0% reduction of blood pressure in rats at 1 mg/kg i.v.

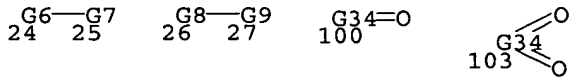
MSTR 5A



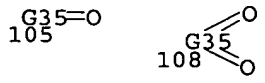
G1 = carbon chain <containing 2-4 C, no triple bonds, unbranched> / 95 / 98



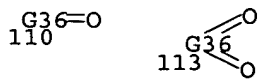
G2 = carbon chain <containing 2-4 C, no triple bonds, unbranched>
G3 = 2 or more H / halo / alkyl <containing 1-3 C> / OH / alkoxy <containing 1-3 C> / alkylsulfonyloxy <containing 1-3 C>
G4 = 1 or more H / halo / alkyl <containing 1-3 C> / OH / alkoxy <containing 1-3 C> / alkylsulfonyloxy <containing 1-3 C>
G5 = alkylene <containing 1-6 C> / 24-11 25-23 / 26-11 27-23 / 100 / 103



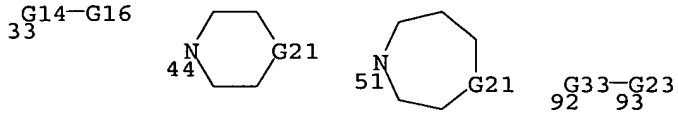
G6 = O / S
G7 = alkylene <containing 2-4 C> (opt. substd. by (1-2) Me) / 105 / **108**



G8 = CH=CH / ethynylene
G9 = alkylene <containing 1-3 C> (opt. substd. by (1-2) Me) / 110 / 113



G11 = NH2 / 33 / pyrrolidino / 44 / 51 / 92



G14 = NH / 35

N——G15
35

G15 = alkyl <containing 1-5 C>
G16 = alkyl <containing 1-10 C> /
cycloalkyl <containing 5-7 C> (opt. substd. by (1-2) G17) /
cycloalkyl <containing 6-15 C, 2-3 rings>
(opt. substd. by (1-2) G17) / 37

G18—G19
37

G17 = alkyl <containing 1-3 C>
G18 = alkylene <containing 1-3 C>
G19 = Ph (opt. substd. by (1-3) G20)
G20 = halo / alkyl <containing 1-3 C> /
alkoxy <containing 1-3 C>
G21 = O / CH2 / 45

N——G22
45

G22 = H / alkyl <containing 1-3 C> /
alkyl <containing 1-3 C> (substd. by 1 or more G24)
G23 = **alkyl <containing 2-3 C>**
(substd. by 1 or more G28) / alkenyl <containing 2-3 C>
(substd. by 1 or more G30)
G24 = 84 / Ph (opt. substd. by (1-3) G27)

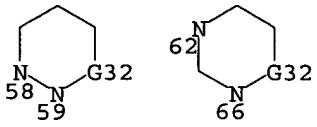
G25—G26
84

G25 = phenylene
G26 = NO2 / CF3
G27 = halo / alkyl <containing 1-3 C> /
alkoxy <containing 1-3 C>
G28 = 88 / OPh (opt. substd. by (1-3) G27)

O——G29—G26
88

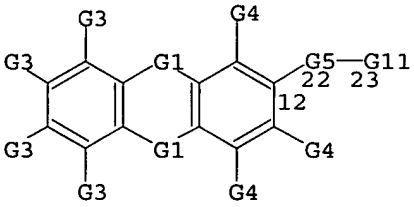
G29 = phenylene
G30 = 89 / Ph (opt. substd. by (1-3) G27)

G31 = phenylene
G32 = **(1-2) CH2**
G33 = **59-22 58-93** / 66-22 62-93

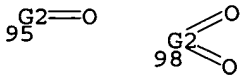


G34 = carbon chain <containing 1-6 C, saturated>
G35 = **carbon chain <containing 2-4 C, saturated>**
G36 = carbon chain <containing 1-3 C, saturated>
Patent location: claim 9
Note: substitution is restricted

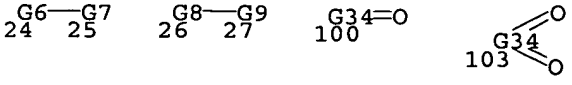
MSTR 5C



G1 = carbon chain <containing 2-4 C, no triple bonds, unbranched> / 95 / 98

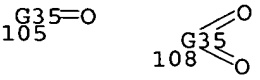


G2 = carbon chain <containing 2-4 C, no triple bonds, unbranched>
G3 = 2 or more H / halo / alkyl <containing 1-3 C> / OH / alkoxy <containing 1-3 C> / alkylsulfonyloxy <containing 1-3 C>
G4 = 1 or more H / halo / alkyl <containing 1-3 C> / OH / alkoxy <containing 1-3 C> / alkylsulfonyloxy <containing 1-3 C>
G5 = alkylene <containing 1-6 C> / 24-12 25-23 / 26-12 27-23 / 100 / 103

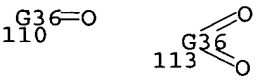


G6 = O / S

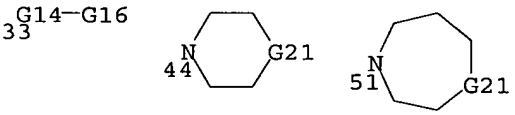
G7 = alkylene <containing 2-4 C>
(opt. substd. by (1-2) Me) / 105 / **108**

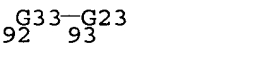


G8 = CH=CH / ethynylene
G9 = alkylene <containing 1-3 C>
(opt. substd. by (1-2) Me) / 110 / 113

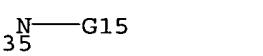


G11 = NH2 / 33 / pyrrolidino / 44 / 51 / 92

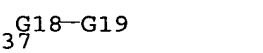




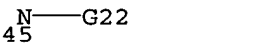
G14 = NH / 35



G15 = alkyl <containing 1-5 C>
G16 = alkyl <containing 1-10 C> /
cycloalkyl <containing 5-7 C> (opt. substd. by (1-2) G17) /
cycloalkyl <containing 6-15 C, 2-3 rings>
(opt. substd. by (1-2) G17) / 37

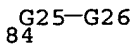


G17 = alkyl <containing 1-3 C>
G18 = alkylene <containing 1-3 C>
G19 = Ph (opt. substd. by (1-3) G20)
G20 = halo / alkyl <containing 1-3 C> /
alkoxy <containing 1-3 C>
G21 = O / CH2 / 45

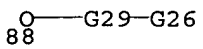


G22 = H / alkyl <containing 1-3 C> /
alkyl <containing 1-3 C> (substd. by 1 or more G24)

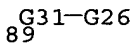
G23 = **alkyl <containing 2-3 C>**
(substd. by 1 or more G28) / alkenyl <containing 2-3 C>
(substd. by 1 or more G30)
G24 = 84 / Ph (opt. substd. by (1-3) G27)



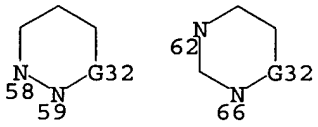
G25 = phenylene
G26 = NO2 / CF3
G27 = halo / alkyl <containing 1-3 C> /
alkoxy <containing 1-3 C>
G28 = 88 / OPh (opt. substd. by (1-3) G27)



G29 = phenylene
G30 = 89 / Ph (opt. substd. by (1-3) G27)

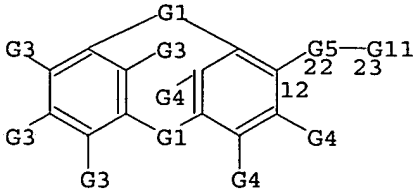


G31 = phenylene
G32 = **(1-2) CH2**
G33 = **59-22 58-93** / 66-22 62-93

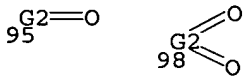


G34 = carbon chain <containing 1-6 C, saturated>
G35 = **carbon chain <containing 2-4 C, saturated>**
G36 = carbon chain <containing 1-3 C, saturated>
Patent location: claim 9
Note: substitution is restricted

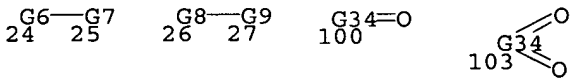
MSTR 5E



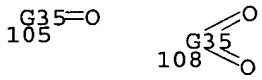
G1 = carbon chain <containing 2-4 C, no triple bonds,
unbranched> / 95 / 98



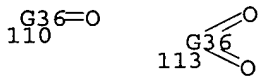
G2 = carbon chain <containing 2-4 C, no triple bonds, unbranched>
G3 = 2 or more H / halo / alkyl <containing 1-3 C> / OH / alkoxy <containing 1-3 C> / alkylsulfonyloxy <containing 1-3 C>
G4 = 1 or more H / halo / alkyl <containing 1-3 C> / OH / alkoxy <containing 1-3 C> / alkylsulfonyloxy <containing 1-3 C>
G5 = alkylene <containing 1-6 C> / 24-12 25-23 / 26-12 27-23 / 100 / 103



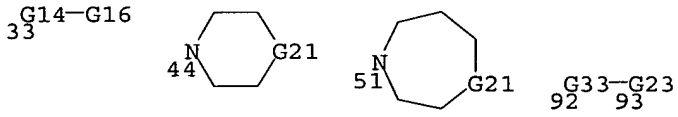
G6 = O / S
G7 = alkylene <containing 2-4 C> (opt. substd. by (1-2) Me) / 105 / **108**



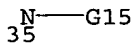
G8 = CH=CH / ethynylene
G9 = alkylene <containing 1-3 C> (opt. substd. by (1-2) Me) / 110 / 113



G11 = NH2 / 33 / pyrrolidino / 44 / 51 / 92



G14 = NH / 35



G15 = alkyl <containing 1-5 C>
G16 = alkyl <containing 1-10 C> / cycloalkyl <containing 5-7 C> (opt. substd. by (1-2) G17) / cycloalkyl <containing 6-15 C, 2-3 rings> (opt. substd. by (1-2) G17) / 37

G18—G19
37

G17 = alkyl <containing 1-3 C>
G18 = alkylene <containing 1-3 C>
G19 = Ph (opt. substd. by (1-3) G20)
G20 = halo / alkyl <containing 1-3 C> /
alkoxy <containing 1-3 C>
G21 = O / CH2 / 45

N——G22
45

G22 = H / alkyl <containing 1-3 C> /
alkyl <containing 1-3 C> (substd. by 1 or more G24)
G23 = **alkyl <containing 2-3 C>**
(substd. by 1 or more G28) / alkenyl <containing 2-3 C>
(substd. by 1 or more G30)
G24 = 84 / Ph (opt. substd. by (1-3) G27)

G25—G26
84

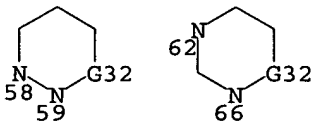
G25 = phenylene
G26 = NO2 / CF3
G27 = halo / alkyl <containing 1-3 C> /
alkoxy <containing 1-3 C>
G28 = 88 / OPh (opt. substd. by (1-3) G27)

O——G29—G26
88

G29 = phenylene
G30 = 89 / Ph (opt. substd. by (1-3) G27)

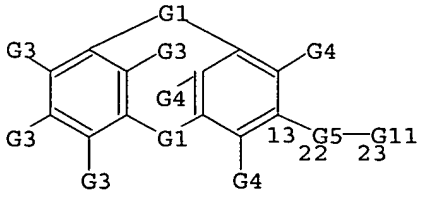
G31—G26
89

G31 = phenylene
G32 = **(1-2) CH2**
G33 = **59-22 58-93** / 66-22 62-93

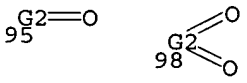


G34 = carbon chain <containing 1-6 C, saturated>
G35 = **carbon chain <containing 2-4 C, saturated>**
G36 = carbon chain <containing 1-3 C, saturated>
Patent location: claim 9
Note: substitution is restricted

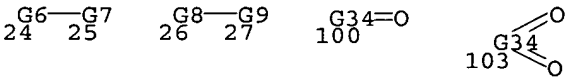
MSTR 5G



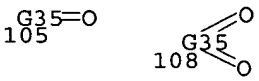
G1 = carbon chain <containing 2-4 C, no triple bonds, unbranched> / 95 / 98



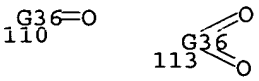
G2 = carbon chain <containing 2-4 C, no triple bonds, unbranched>
G3 = 2 or more H / halo / alkyl <containing 1-3 C> / OH / alkoxy <containing 1-3 C> / alkylsulfonyloxy <containing 1-3 C>
G4 = 1 or more H / halo / alkyl <containing 1-3 C> / OH / alkoxy <containing 1-3 C> / alkylsulfonyloxy <containing 1-3 C>
G5 = alkylene <containing 1-6 C> / 24-13 25-23 / 26-13 27-23 / 100 / 103



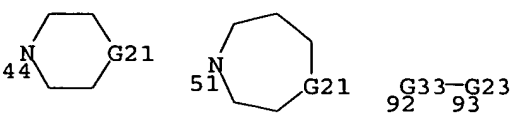
G6 = O / S
G7 = alkylene <containing 2-4 C> (opt. substd. by (1-2) Me) / 105 / **108**



G8 = CH=CH / ethynylene
G9 = alkylene <containing 1-3 C> (opt. substd. by (1-2) Me) / 110 / 113



G11 = NH2 / 33 / pyrrolidino / 44 / 51 / 92



G14 = NH / 35

N——G15
35

G15 = alkyl <containing 1-5 C>
G16 = alkyl <containing 1-10 C> /
cycloalkyl <containing 5-7 C> (opt. substd. by (1-2) G17) /
cycloalkyl <containing 6-15 C, 2-3 rings>
(opt. substd. by (1-2) G17) / 37

G18—G19
37

G17 = alkyl <containing 1-3 C>
G18 = alkylene <containing 1-3 C>
G19 = Ph (opt. substd. by (1-3) G20)
G20 = halo / alkyl <containing 1-3 C> /
alkoxy <containing 1-3 C>
G21 = O / CH2 / 45

N——G22
45

G22 = H / alkyl <containing 1-3 C> /
alkyl <containing 1-3 C> (substd. by 1 or more G24)
G23 = **alkyl <containing 2-3 C>**
(substd. by 1 or more G28) / alkenyl <containing 2-3 C>
(substd. by 1 or more G30)
G24 = 84 / Ph (opt. substd. by (1-3) G27)

G25—G26
84

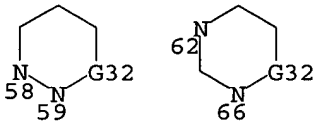
G25 = phenylene
G26 = NO2 / CF3
G27 = halo / alkyl <containing 1-3 C> /
alkoxy <containing 1-3 C>
G28 = 88 / OPh (opt. substd. by (1-3) G27)

O——G29—G26
88

G29 = phenylene
G30 = 89 / Ph (opt. substd. by (1-3) G27)

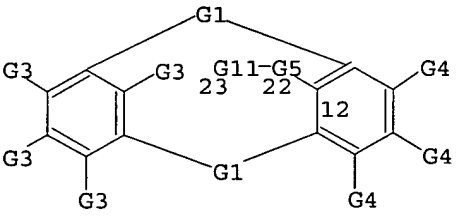
G31—G26
89

G31 = phenylene
G32 = **(1-2) CH2**
G33 = **59-22 58-93** / 66-22 62-93

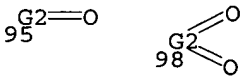


G34 = carbon chain <containing 1-6 C, saturated>
G35 = **carbon chain <containing 2-4 C, saturated>**
G36 = carbon chain <containing 1-3 C, saturated>
Patent location: claim 9
Note: substitution is restricted

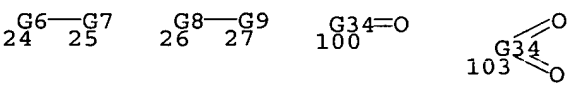
MSTR 5I



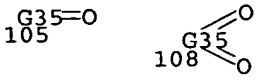
G1 = carbon chain <containing 2-4 C, no triple bonds, unbranched> / 95 / 98



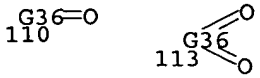
G2 = carbon chain <containing 2-4 C, no triple bonds, unbranched>
G3 = 2 or more H / halo / alkyl <containing 1-3 C> / OH / alkoxy <containing 1-3 C> / alkylsulfonyloxy <containing 1-3 C>
G4 = 1 or more H / halo / alkyl <containing 1-3 C> / OH / alkoxy <containing 1-3 C> / alkylsulfonyloxy <containing 1-3 C>
G5 = alkylene <containing 1-6 C> / 24-12 25-23 / 26-12 27-23 / 100 / 103



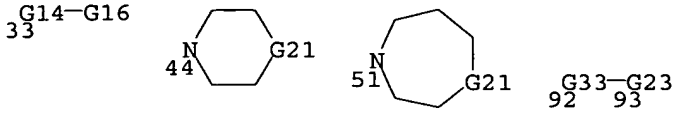
G6 = O / S
G7 = alkylene <containing 2-4 C> (opt. substd. by (1-2) Me) / 105 / **108**



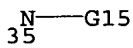
G8 = CH=CH / ethynylene
G9 = alkylene <containing 1-3 C>
(opt. substd. by (1-2) Me) / 110 / 113



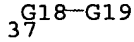
G11 = NH2 / 33 / pyrrolidino / 44 / 51 / 92



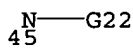
G14 = NH / 35



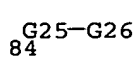
G15 = alkyl <containing 1-5 C>
G16 = alkyl <containing 1-10 C> /
cycloalkyl <containing 5-7 C> (opt. substd. by (1-2) G17) /
cycloalkyl <containing 6-15 C, 2-3 rings>
(opt. substd. by (1-2) G17) / 37



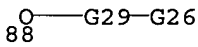
G17 = alkyl <containing 1-3 C>
G18 = alkylene <containing 1-3 C>
G19 = Ph (opt. substd. by (1-3) G20)
G20 = halo / alkyl <containing 1-3 C> /
alkoxy <containing 1-3 C>
G21 = O / CH2 / 45



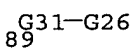
G22 = H / alkyl <containing 1-3 C> /
alkyl <containing 1-3 C> (substd. by 1 or more G24)
G23 = **alkyl <containing 2-3 C>**
(substd. by 1 or more G28) / alkenyl <containing 2-3 C>
(substd. by 1 or more G30)
G24 = 84 / Ph (opt. substd. by (1-3) G27)



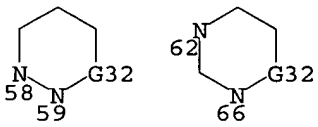
G25 = phenylene
G26 = NO2 / CF3
G27 = halo / alkyl <containing 1-3 C> / alkoxy <containing 1-3 C>
G28 = 88 / OPh (opt. substd. by (1-3) G27)



G29 = phenylene
G30 = 89 / Ph (opt. substd. by (1-3) G27)

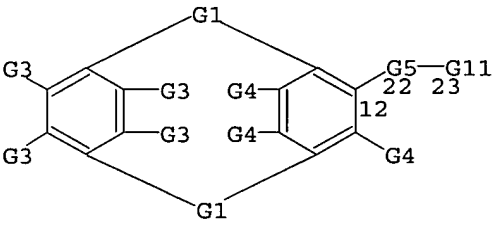


G31 = phenylene
G32 = **(1-2) CH2**
G33 = **59-22 58-93** / 66-22 62-93

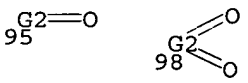


G34 = carbon chain <containing 1-6 C, saturated>
G35 = **carbon chain <containing 2-4 C, saturated>**
G36 = carbon chain <containing 1-3 C, saturated>
Patent location: claim 9
Note: substitution is restricted

MSTR 5K



G1 = carbon chain <containing 2-4 C, no triple bonds, unbranched> / 95 / 98

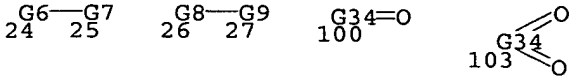


G2 = carbon chain <containing 2-4 C, no triple bonds, unbranched>
G3 = 2 or more H / halo / alkyl <containing 1-3 C> / OH /

alkoxy <containing 1-3 C> / alkylsulfonyloxy <containing 1-3 C>

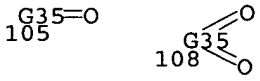
G4 = 1 or more H / halo / alkyl <containing 1-3 C> / OH / alkoxy <containing 1-3 C> / alkylsulfonyloxy <containing 1-3 C>

G5 = alkylene <containing 1-6 C> / 24-12 25-23 / 26-12 27-23 / 100 / 103



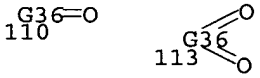
G6 = O / S

G7 = alkylene <containing 2-4 C> (opt. substd. by (1-2) Me) / 105 / **108**

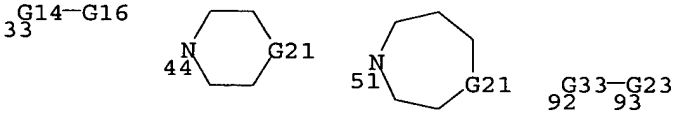


G8 = CH=CH / ethynylene

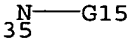
G9 = alkylene <containing 1-3 C> (opt. substd. by (1-2) Me) / 110 / 113



G11 = NH2 / 33 / pyrrolidino / 44 / 51 / 92

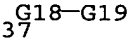


G14 = NH / 35



G15 = alkyl <containing 1-5 C>

G16 = alkyl <containing 1-10 C> / cycloalkyl <containing 5-7 C> (opt. substd. by (1-2) G17) / cycloalkyl <containing 6-15 C, 2-3 rings> (opt. substd. by (1-2) G17) / 37



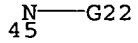
G17 = alkyl <containing 1-3 C>

G18 = alkylene <containing 1-3 C>

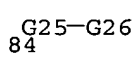
G19 = Ph (opt. substd. by (1-3) G20)

G20 = halo / alkyl <containing 1-3 C> /

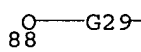
alkoxy <containing 1-3 C>
G21 = O / CH2 / 45



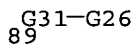
G22 = H / alkyl <containing 1-3 C> /
alkyl <containing 1-3 C> (substd. by 1 or more G24)
G23 = **alkyl <containing 2-3 C>**
(substd. by 1 or more G28) / alkenyl <containing 2-3 C>
(substd. by 1 or more G30)
G24 = 84 / Ph (opt. substd. by (1-3) G27)



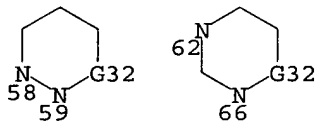
G25 = phenylene
G26 = NO2 / CF3
G27 = halo / alkyl <containing 1-3 C> /
alkoxy <containing 1-3 C>
G28 = 88 / OPh (opt. substd. by (1-3) G27)



G29 = phenylene
G30 = 89 / Ph (opt. substd. by (1-3) G27)



G31 = phenylene
G32 = **(1-2) CH2**
G33 = **59-22 58-93** / 66-22 62-93



G34 = carbon chain <containing 1-6 C, saturated>
G35 = **carbon chain <containing 2-4 C, saturated>**
G36 = carbon chain <containing 1-3 C, saturated>
Patent location: claim 9
Note: substitution is restricted

BEILSTEIN (2 ~~hits~~ references) - narrowest structure


```
=> file beilstein
FILE 'BEILSTEIN' ENTERED AT 12:01:28 ON 19 OCT 2005
COPYRIGHT (c) 2005 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften
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FILE LAST UPDATED ON OCTOBER 10, 2005

FILE COVERS 1771 TO 2005.
*** FILE CONTAINS  9,363,954 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in
   separate documents and can not be searched together in one query.
   Reaction data for BEILSTEIN compounds may be displayed
   immediately with the display codes PRE (preparations) and REA
   (reactions).  A substance answer set retrieved after the search
   for a chemical name, a compounds with available reaction
   information by combining with PRE/FA, REA/FA or more generally
   with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
   between a BEILSTEIN compound and belonging reactions. For mo
   detailed reaction searches BRNs can be searched as reaction
   partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE  <<<

**********************************************************************
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.                 *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE    *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE           *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                         *
* FOR PRICE INFORMATION SEE HELP COST                                 *
**********************************************************************
    NEW
* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE
  SEARCHED, SELECTED AND TRANSFERRED.
* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES,
  ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A
  COMPOUND AT A GLANCE.

=> d stat que L52
L42             STR
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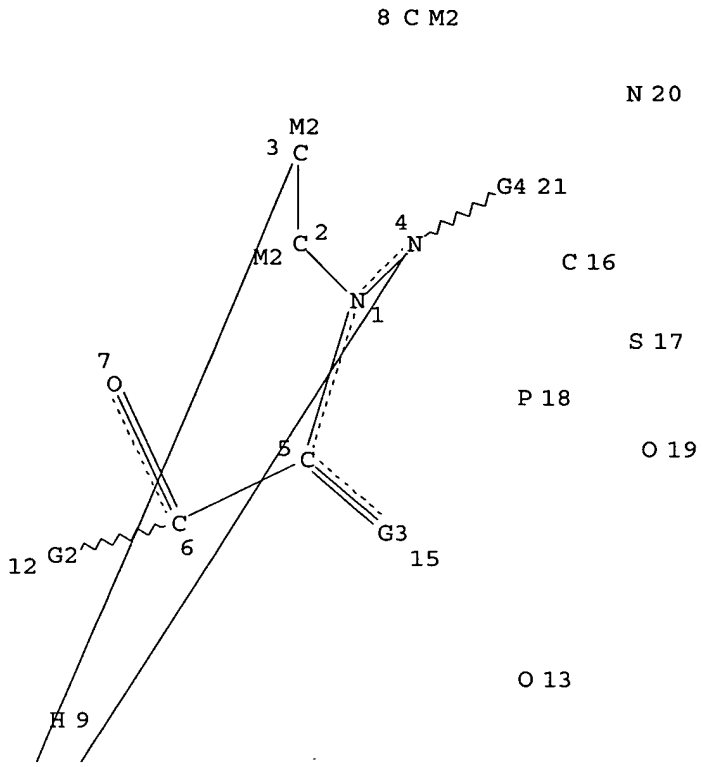
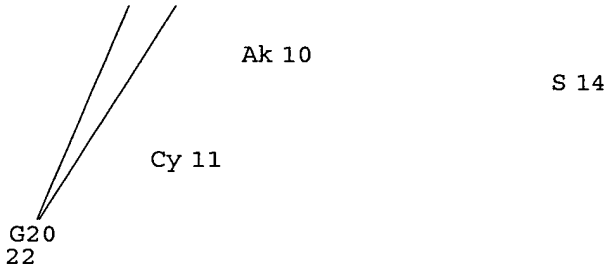


Page 1-A



Page 2-A
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VAR G3=13/14
VAR G4=16/17/18/19/20
REP G20=(1-3) 8-4 8-3
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HCOUNT	IS M2	AT	3
HCOUNT	IS M2	AT	8
NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS C	AT	5
NSPEC	IS C	AT	6
NSPEC	IS C	AT	7
NSPEC	IS R	AT	8

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NSPEC   IS C       AT  10
NSPEC   IS C       AT  11
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NSPEC   IS C       AT  14
NSPEC   IS C       AT  15
NSPEC   IS RC      AT  16
NSPEC   IS RC      AT  17
NSPEC   IS RC      AT  18
NSPEC   IS RC      AT  19
NSPEC   IS RC      AT  20
NSPEC   IS C       AT  21
NSPEC   IS R       AT  22
CONNECT IS E3  RC AT   5
CONNECT IS X3  RC AT   6
CONNECT IS E1  RC AT   7
CONNECT IS E1  RC AT  13
CONNECT IS E1  RC AT  14
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT   5  6  7  9 10 13 14 16 17 18 19 20
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  22

STEREO ATTRIBUTES: NONE
L43          20 SEA FILE=BEILSTEIN SSS FUL L42
L50          73 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  6433892/BABSAN
L52          19 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L43 AND L50
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All 19 are from the same reference

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=> d que nos L53
L42             STR
L43          20 SEA FILE=BEILSTEIN SSS FUL L42
L50          73 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  6433892/BABSAN
L52          19 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L43 AND L50
L53           1 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L43 NOT L52


=> d L52 ide allref 1; d L53 ide allref 1


L52  ANSWER 1 OF 19 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

     Beilstein Records (BRN):        9661119
     Chemical Name (CN):             3,3-dimethyl-1-<2-(6-(3-pyridyl)hex-5-
                                     ynoyl)perhydropyridazin-1-yl>pentane-1,2-
                                     dione
     Autonom Name (AUN):             3,3-dimethyl-1-<2-(6-pyridin-3-yl-hex-5-
                                     ynoyl)-tetrahydro-pyridazin-1-yl>-pentane-
                                     1,2-dione
     Molec. Formula (MF):            C22 H29 N3 O3
     Molecular Weight (MW):          383.49
     Lawson Number (LN):             28000, 26377, 2339
     Compound Type (CTYPE):          heterocyclic
     Constitution ID (CONSID):       8143712
     Tautomer ID (TAUTID):           9045841
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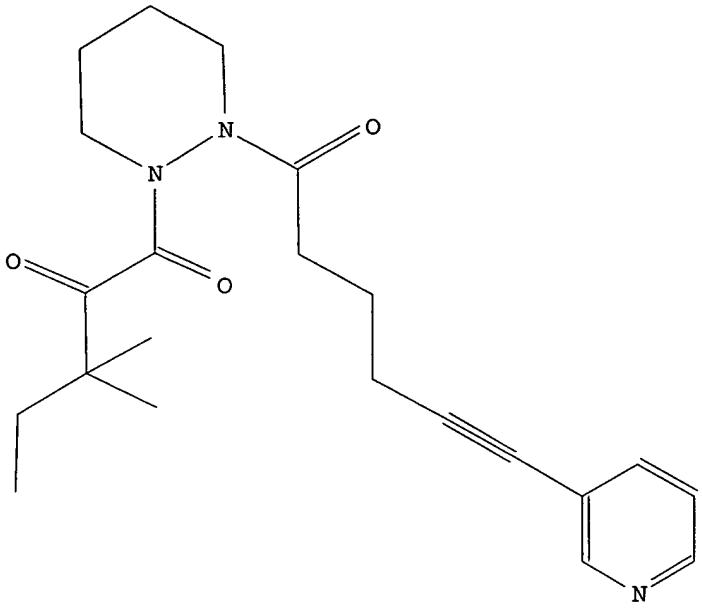
Entry Date (DED): 2004/07/21
Update Date (DUPD): 2004/07/21



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AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
CPD	Crystal Property Description	1
NMR	Nuclear Magnetic Resonance	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

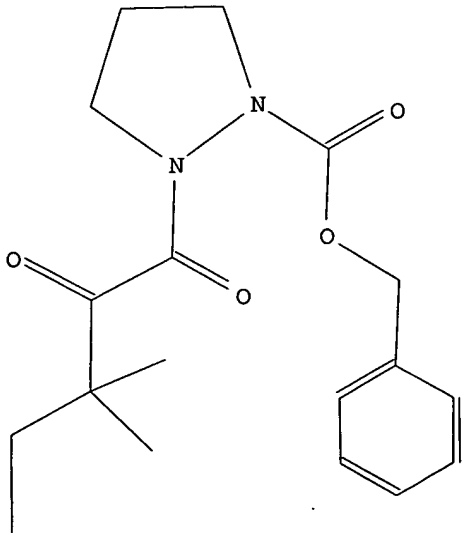
All References:
ALLREF

1. Wilkinson, Douglas E.; Thomas, Bert E.; Limburg, David C.; Holmes, Agnes; Sauer, Hansjorg; Ross, Douglas T.; Soni, Raj; Chen, Yi; Guo, Hong; Howorth, Pamela; Valentine, Heather; et al., Bioorg.Med.Chem., CODEN: BMECEP, 11, <2003>, 4815 - 4826; BABS-6433892

(there are 18 other structures [hits] that have the same reference)

L53 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Beilstein Records (BRN):	9644844
Chemical Name (CN):	2-(3,3-dimethyl-2-oxo-pentanoyl)-pyrazolidine-1-carboxylic acid benzyl ester
Autonom Name (AUN):	2-(3,3-dimethyl-2-oxo-pentanoyl)-pyrazolidine-1-carboxylic acid benzyl ester
Molec. Formula (MF):	C18 H24 N2 O4
Molecular Weight (MW):	332.40
Lawson Number (LN):	28004, 5228, 2339, 1762
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	8129638
Tautomer ID (TAUTID):	9024959
Entry Date (DED):	2004/07/21
Update Date (DUPD):	2004/07/21



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1

CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	4
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Wilkinson, Douglas E.; Thomas, Bert E.; Limburg, David C.; Holmes, Agnes; Sauer, Hansjorg; Ross, Douglas T.; Soni, Raj; Chen, Yi; Guo, Hong; Howorth, Pamela; Valentine, Heather; et al., Bioorg.Med.Chem., CODEN: BMECEP, 11, <2003>, 4815 - 4826; BABS-6433892

AUTHOR Search


```
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FILE COVERS 1907 - 19 Oct 2005  VOL 143 ISS 17
FILE LAST UPDATED: 18 Oct 2005  (20051018/ED)

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=> d que L57
L54          734 SEA FILE=CAPLUS ABB=ON  PLU=ON  HAMILTON G?/AU
L55         7835 SEA FILE=CAPLUS ABB=ON  PLU=ON  HUANG W?/AU
L56        16214 SEA FILE=CAPLUS ABB=ON  PLU=ON  WU Y?/AU
L57            4 SEA FILE=CAPLUS ABB=ON  PLU=ON  L54 AND L55 AND L56


=> file medline embase
FILE 'MEDLINE' ENTERED AT 13:00:08 ON 19 OCT 2005

FILE 'EMBASE' ENTERED AT 13:00:08 ON 19 OCT 2005
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=> d que L65
L62         1169 SEA HAMILTON G/AU OR HAMILTON G ?/AU OR HAMILTON GR?/AU
L63         4309 SEA HUANG W?/AU
L64         8108 SEA WU Y?/AU
L65            2 SEA L62 AND L63 AND L64


=> dup rem L57 L65
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FILE 'EMBASE' ENTERED AT 13:00:25 ON 19 OCT 2005
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PROCESSING COMPLETED FOR L57
PROCESSING COMPLETED FOR L65
L66            4 DUP REM L57 L65 (2 DUPLICATES REMOVED)
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ANSWERS '1-4' FROM FILE CAPLUS

=> d ibib abs hitind L66 1-4

L66 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2002:515544 CAPLUS
DOCUMENT NUMBER: 137:201562
TITLE: Synthesis of N-Glyoxyl Prolyl and Pipecolyl Amides and Thioesters and Evaluation of Their In Vitro and In Vivo Nerve Regenerative Effects
AUTHOR(S): **Hamilton, Gregory S.**; **Wu, Yong-Qian**; Limburg, David C.; Wilkinson, Douglas E.; Vaal, Mark J.; Li, Jia-He; Thomas, Christine; **Huang, Wei**; Sauer, Hansjorg; Ross, Douglas T.; Soni, Raj; Chen, Yi; Guo, Hongshi; Howorth, Pamela; Valentine, Heather; Liang, Shi; Spicer, Dawn; Fuller, Mike; Steiner, Joseph P.
CORPORATE SOURCE: Department of Research, Guilford Pharmaceuticals Inc., Baltimore, MD, 21224, USA
SOURCE: Journal of Medicinal Chemistry (2002), 45(16), 3549-3557
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:201562
AB The recent discovery that small mol. ligands for the peptidyl-prolyl isomerase (PPIase) FKBP12 possess powerful neuroprotective and neuroregenerative properties in vitro and in vivo suggests therapeutic utility for such compds. in neurodegenerative disease. The neurotrophic effects of these compds. are independent of the immunosuppressive pathways by which drugs such as FK506 and rapamycin operate. Previous work by the authors and other groups exploring the structure-activity relationships (SAR) of small mols. that mimic only the FKBP binding domain portion of FK506 has focused on esters of proline and pipecolic acid. The authors have explored amide and thioester analogs of these earlier structures and found that they too are extremely potent in promoting recovery of lesioned dopaminergic pathways in a mouse model of Parkinson's disease. Several compds. were shown to be highly effective upon oral administration after lesioning of the dopaminergic pathway, providing further evidence of the potential clin. utility of a variety of structural classes of FKBP12 ligands.
CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 7
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L66 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:172490 CAPLUS
DOCUMENT NUMBER: 136:232310
TITLE: Preparation of N-substituted cyclic aza compounds having neuronal activity
INVENTOR(S): **Wu, Yong-qian**; **Huang, Wei**; **Hamilton, Gregory S.**
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 54 pp., Cont.-in-part of U. S. Ser. No. 551,618.
CODEN: USXXCO
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002028814	A1	20020307	US 2001-835523	20010417
US 6417189	B1	20020709	US 2000-551618	20000417
PRIORITY APPLN. INFO.:			US 1999-164950P	P 19991112
			US 2000-551618	A2 20000417

OTHER SOURCE(S): MARPAT 136:232310
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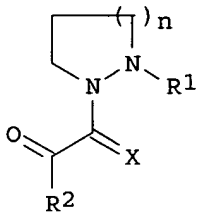

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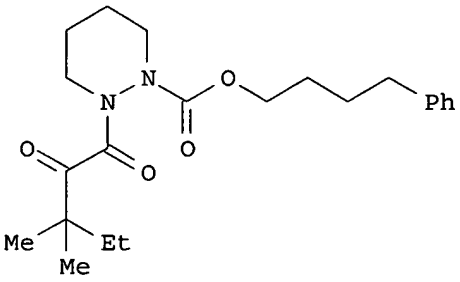


II

AB Title compds. I [n = 1-3; R1 = CR3, CO2R3, COR3, etc.; R2, R3 = H, alkyl, alkenyl, etc.; X = O, S], useful for effecting neuronal activities, were prepared Thus, II was prepared via a multi-step synthesis from tert-Bu 2-benzylperhydropyridazinecarboxylate. Biol. data for I (results of test for rotamase inhibition and MPTP model of Parkinson's disease) were given. E.g., II possessed a Ki value of 1175 nM in inhibition studies of rotamase and a 14% TH recovery in MPTP models.

IC ICM C07D413-02
ICS C07D043-02; A61K031-675; A61K031-551; A61K031-501; A61K031-50; A61K031-4245; A61K031-4155
INCL 514249000
CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

L66 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:780859 CAPLUS
DOCUMENT NUMBER: 135:331433
TITLE: Preparation of cyclic diaza compounds for treating

neurodegenerative disorders

INVENTOR(S): **Wu, Yong-Qian; Huang, Wei; Hamilton, Gregory S.**

PATENT ASSIGNEE(S): GPI NIL Holdings, Inc., USA

SOURCE: PCT Int. Appl., 162 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

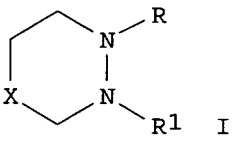
FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001079177	A1	20011025	WO 2001-US12322	20010417
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6417189	B1	20020709	US 2000-551618	20000417
PRIORITY APPLN. INFO.:			US 2000-551618 A	20000417
			US 1999-164950P P	19991112

OTHER SOURCE(S): MARPAT 135:331433

GI



I

AB Title compds. [I;X = bond, CH2; R = COY(CH2)nC6H5, 5-(3-pyridyl)-pent-4-ynoyl, NCCCCH2CH2CO, 5-(3-pyridyl)-pentanoyl, 3-(3-pyridyl)-propoxycarbonyl; Y = O, bond; n = 5, 4, 3, 2; R1 = C6H5CH2SO2, (CH3CH2)(CH3)2CCOCO, C6H5CH2SO2, cyclohexylaminocarbonyl] are prepared for pharmaceutical compns. comprising such compds. and methods of their use for effecting neuronal activities. Thus, the title compound I (X = bond; Y = bond; n = 4; R = COY(CH2)nC6H5; R1 = (CH3CH2)(CH3)2CCOCO) was prepared and biol. tested in mice for MPTP model of Parkinson's disease and showed recovery of TH-stained dopaminergic neurons.

IC ICM C07D231-04
ICS C07D401-06; C07D401-12; C07D237-04; C07D487-04; A61K031-415; A61K031-50; A61P025-00

CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L66 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:380557 CAPLUS

DOCUMENT NUMBER: 134:366884

TITLE: Preparation of N-substituted cyclic aza compounds

having neuronal activity
INVENTOR(S): **Wu, Yong-Qian; Huang, Wei; Hamilton, Gregory S.**
PATENT ASSIGNEE(S): GPI Nil Holdings, Inc., USA
SOURCE: PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2001036388	A1	20010525	WO 2000-US23603		20000828
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
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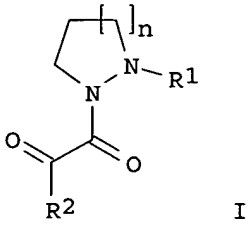
CA 2390071	AA	20010525	CA 2000-2390071		20000828
EP 1242383	A1	20020925	EP 2000-957870		20000828
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL					
JP 2003514799	T2	20030422	JP 2001-538878		20000828
AU 781740	B2	20050609	AU 2000-69428		20000828
PRIORITY APPLN. INFO.:			US 1999-164950P	P	19991112
			US 2000-551618	A	20000417
			WO 2000-US23603	W	20000828

OTHER SOURCE(S): MARPAT 134:366884
GI



I

AB The title compds. [I; n = 1-3; R1 = CR3, CO2R3, COR3, etc.; R2, R3 = H, alkyl, alkenyl, etc.; X = O, S], useful for effecting neuronal activities, were prepared E.g., a multi-step synthesis of I [n = 2; R1 = CO2(CH2)4Ph; R2 = CMe2Et; X = O] was described. Biol. data for compds. I (results of test for rotamase inhibition and MPTP model of Parkinson's disease) were given.

IC ICM C07D231-04
ICS C07D401-06; C07D401-12; C07D237-04; C07D487-04
CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Search history

Truong 09_835523 10/19/2005

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> d his full

     (FILE 'HOME' ENTERED AT 09:26:46 ON 19 OCT 2005)

     FILE 'REGISTRY' ENTERED AT 09:26:52 ON 19 OCT 2005
L1             STRUCTURE UPLOADED
L2           6 SEA SSS SAM L1

     FILE 'CAPLUS' ENTERED AT 09:27:37 ON 19 OCT 2005
L3           7 SEA ABB=ON  PLU=ON  L2

     FILE 'STNGUIDE' ENTERED AT 09:27:57 ON 19 OCT 2005

     FILE 'REGISTRY' ENTERED AT 09:28:45 ON 19 OCT 2005
               D SCA L2

     FILE 'STNGUIDE' ENTERED AT 09:29:54 ON 19 OCT 2005

     FILE 'CAPLUS' ENTERED AT 09:31:04 ON 19 OCT 2005
               E US2001-835523/APPS
L4           1 SEA ABB=ON  PLU=ON  US2001-835523/AP
               SEL RN

     FILE 'REGISTRY' ENTERED AT 09:31:31 ON 19 OCT 2005
L5          46 SEA ABB=ON  PLU=ON  (110-52-1/BI OR 1120-90-7/BI OR 1939-99-7/B
               I OR 2270-20-4/BI OR 28276-08-6/BI OR 3173-53-3/BI OR 340255-68
               -7/BI OR 340255-88-1/BI OR 340255-89-2/BI OR 340255-90-5/BI OR
               340255-91-6/BI OR 340255-92-7/BI OR 340255-93-8/BI OR 340255-94
               -9/BI OR 340255-95-0/BI OR 340255-96-1/BI OR 340255-97-2/BI OR
               340255-98-3/BI OR 340255-99-4/BI OR 340256-00-0/BI OR 340256-01
               -1/BI OR 340256-02-2/BI OR 340256-03-3/BI OR 340256-04-4/BI OR
               340256-05-5/BI OR 340256-06-6/BI OR 340256-07-7/BI OR 340256-08
               -8/BI OR 340256-09-9/BI OR 340256-10-2/BI OR 340256-11-3/BI OR
               340256-12-4/BI OR 340256-13-5/BI OR 340256-14-6/BI OR 340256-15
               -7/BI OR 340256-16-8/BI OR 340256-17-9/BI OR 340256-18-0/BI OR
               340256-19-1/BI OR 340256-20-4/BI OR 340256-21-5/BI OR 53293-00-
               8/BI OR 5331-43-1/BI OR 53370-84-6/BI OR 5781-53-3/BI OR
               95076-93-0/BI)
               D SCA

     FILE 'STNGUIDE' ENTERED AT 09:32:00 ON 19 OCT 2005
               D SCA L2

     FILE 'REGISTRY' ENTERED AT 09:35:23 ON 19 OCT 2005
               D SCA L2

     FILE 'STNGUIDE' ENTERED AT 09:35:30 ON 19 OCT 2005

     FILE 'CAPLUS' ENTERED AT 09:37:19 ON 19 OCT 2005

     FILE 'REGISTRY' ENTERED AT 09:37:21 ON 19 OCT 2005
L6             STRUCTURE UPLOADED
L7          11 SEA SSS SAM L6
L8           5 SEA ABB=ON  PLU=ON  L7 NOT L2
               D SCA

     FILE 'STNGUIDE' ENTERED AT 09:39:05 ON 19 OCT 2005

     FILE 'CAPLUS' ENTERED AT 09:44:25 ON 19 OCT 2005
```

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L9          12 SEA ABB=ON  PLU=ON  L7

     FILE 'REGISTRY' ENTERED AT 09:45:23 ON 19 OCT 2005

     FILE 'STNGUIDE' ENTERED AT 09:45:52 ON 19 OCT 2005

     FILE 'REGISTRY' ENTERED AT 09:47:00 ON 19 OCT 2005
L10         76 SEA SSS FUL L1
               SAVE L10 TRU523STRA/A

     FILE 'CAPLUS' ENTERED AT 09:48:04 ON 19 OCT 2005
L11         21 SEA ABB=ON  PLU=ON  L10

     FILE 'REGISTRY' ENTERED AT 09:48:24 ON 19 OCT 2005
               D SCA L10

     FILE 'STNGUIDE' ENTERED AT 09:56:00 ON 19 OCT 2005

     FILE 'MARPAT' ENTERED AT 09:57:31 ON 19 OCT 2005
L12         16 SEA SSS SAM L1
L13          5 SEA ABB=ON  PLU=ON  L11 NOT L12
L14         16 SEA ABB=ON  PLU=ON  L12 NOT L11

     FILE 'BEILSTEIN' ENTERED AT 09:59:21 ON 19 OCT 2005
L15         53 SEA SSS FUL L1
L16          4 SEA ABB=ON  PLU=ON  L15 AND RN/FA

     FILE 'STNGUIDE' ENTERED AT 10:01:19 ON 19 OCT 2005

     FILE 'BEILSTEIN' ENTERED AT 10:02:51 ON 19 OCT 2005
L17             STRUCTURE UPLOADED
L18         25 SEA SSS FUL L17

     FILE 'MARPAT' ENTERED AT 10:04:47 ON 19 OCT 2005
L19          1 SEA SSS SAM L17
L20          1 SEA ABB=ON  PLU=ON  L19 NOT L11
L21            STRUCTURE UPLOADED
L22          0 SEA SSS SAM L21

     FILE 'BEILSTEIN' ENTERED AT 10:12:09 ON 19 OCT 2005
L23         21 SEA SSS FUL L21
L24          1 SEA ABB=ON  PLU=ON  L23 AND RN/FA
L25          0 SEA ABB=ON  PLU=ON  L23 AND REF/FA
L26          0 SEA ABB=ON  PLU=ON  L23 AND XREF/FA
L27          0 SEA ABB=ON  PLU=ON  L23 AND ALLREF/FA

     FILE 'MARPAT' ENTERED AT 10:14:53 ON 19 OCT 2005
L28         17 SEA SSS FUL L21

     FILE 'CAPLUS, MARPAT' ENTERED AT 10:16:23 ON 19 OCT 2005
L29         34 DUP REM L11 L28 (4 DUPLICATES REMOVED)
                    ANSWERS '1-21' FROM FILE CAPLUS
                    ANSWERS '22-34' FROM FILE MARPAT
               D SCA L28

     FILE 'STNGUIDE' ENTERED AT 10:22:07 ON 19 OCT 2005

     FILE 'BEILSTEIN' ENTERED AT 10:26:14 ON 19 OCT 2005
L30             STRUCTURE UPLOADED
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L31          20 SEA SSS FUL L30
L32           0 SEA ABB=ON  PLU=ON  L31 AND ED/FA
                D IDE L31 1
L33       11685 SEA ABB=ON  PLU=ON  HAMILTON?/AU
L34           0 SEA ABB=ON  PLU=ON  L31 AND L33
L35       64396 SEA ABB=ON  PLU=ON  HUANG?/AU
L36           0 SEA ABB=ON  PLU=ON  L35 AND L31
L37          38 SEA ABB=ON  PLU=ON  HAMILT?
L38           0 SEA ABB=ON  PLU=ON  L37 AND L31

     FILE 'MARPAT' ENTERED AT 10:34:13 ON 19 OCT 2005
L39           0 SEA SUB=L28 SSS SAM L30
L40          14 SEA SUB=L28 SSS FUL L30

     FILE 'REGISTRY' ENTERED AT 10:35:52 ON 19 OCT 2005

     FILE 'CAPLUS' ENTERED AT 10:35:54 ON 19 OCT 2005
                D STAT QUE L11
                D IBIB ABS HITSTR L11 1-21

     FILE 'MARPAT' ENTERED AT 10:40:15 ON 19 OCT 2005

     FILE 'MARPAT' ENTERED AT 10:40:30 ON 19 OCT 2005
                D STAT QUE L40

     FILE 'CAPLUS, MARPAT' ENTERED AT 10:40:54 ON 19 OCT 2005
L41          32 DUP REM L11 L40 (3 DUPLICATES REMOVED)
                     ANSWERS '1-21' FROM FILE CAPLUS
                     ANSWERS '22-32' FROM FILE MARPAT
                D IBIB ABS HIT 22-32 L41

     FILE 'STNGUIDE' ENTERED AT 10:43:58 ON 19 OCT 2005

     FILE 'BEILSTEIN' ENTERED AT 10:49:21 ON 19 OCT 2005
L42             STRUCTURE UPLOADED
L43          20 SEA SSS FUL L42
                D L43 1 ALLREF
L44         146 SEA ABB=ON  PLU=ON  BERT?
L45           0 SEA ABB=ON  PLU=ON  L43 AND L44
L46           0 SEA ABB=ON  PLU=ON  BERT?/ALLREF
L47           0 SEA ABB=ON  PLU=ON  BERT?/REF
L48           0 SEA ABB=ON  PLU=ON  BERT?/XREF

     FILE 'STNGUIDE' ENTERED AT 10:53:10 ON 19 OCT 2005

     FILE 'MARPAT' ENTERED AT 11:06:03 ON 19 OCT 2005
                SAVE L40 TRU523MARP/A
                D SAV

     FILE 'BEILSTEIN' ENTERED AT 11:53:44 ON 19 OCT 2005
                SEL BABSAN L43
L49          19 SEA ABB=ON  PLU=ON  L43 AND BABSAN/FA
L50          73 SEA ABB=ON  PLU=ON  6433892/BABSAN
L51           1 SEA ABB=ON  PLU=ON  L43 NOT L50

     FILE 'BEILSTEIN' ENTERED AT 11:58:46 ON 19 OCT 2005
                D STAT QUE L31
L52          19 SEA ABB=ON  PLU=ON  L43 AND L50
L53           1 SEA ABB=ON  PLU=ON  L43 NOT L52
```

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     FILE 'BEILSTEIN' ENTERED AT 12:01:28 ON 19 OCT 2005
               D STAT QUE L52
               D QUE NOS L53
               D L52 IDE ALLREF 1
               D L53 IDE ALLREF 1

     FILE 'STNGUIDE' ENTERED AT 12:07:37 ON 19 OCT 2005
               D COST FULL

     FILE 'CAPLUS' ENTERED AT 12:50:19 ON 19 OCT 2005
L54          734 SEA ABB=ON  PLU=ON  HAMILTON G?/AU
L55         7835 SEA ABB=ON  PLU=ON  HUANG W?/AU
L56        16214 SEA ABB=ON  PLU=ON  WU Y?/AU
L57            4 SEA ABB=ON  PLU=ON  L54 AND L55 AND L56

     FILE 'CAPLUS' ENTERED AT 12:51:31 ON 19 OCT 2005
               D QUE L57
L58          133 SEA ABB=ON  PLU=ON  (L54 AND (L55 OR L56)) OR (L55 AND L56)
L59           50 SEA ABB=ON  PLU=ON  (L54 AND (L55 OR L56))
               E HAMILTON G/AU
L60          404 SEA ABB=ON  PLU=ON  HAMILTON G/AU OR HAMILTON G ?/AU OR
               HAMILTON GR?/AU
L61           50 SEA ABB=ON  PLU=ON  L60 AND (L55 OR L56)

     FILE 'CAPLUS' ENTERED AT 12:56:49 ON 19 OCT 2005
               D QUE L57
               D IBIB ABS HITIND L57 1-4

     FILE 'MEDLINE, EMBASE' ENTERED AT 12:58:21 ON 19 OCT 2005
L62         1169 SEA ABB=ON  PLU=ON  HAMILTON G/AU OR HAMILTON G ?/AU OR
               HAMILTON GR?/AU
L63         4309 SEA ABB=ON  PLU=ON  HUANG W?/AU
L64         8108 SEA ABB=ON  PLU=ON  WU Y?/AU
L65            2 SEA ABB=ON  PLU=ON  L62 AND L63 AND L64

     FILE 'STNGUIDE' ENTERED AT 12:59:39 ON 19 OCT 2005

     FILE 'CAPLUS' ENTERED AT 12:59:43 ON 19 OCT 2005
               D QUE L57

     FILE 'MEDLINE, EMBASE' ENTERED AT 13:00:08 ON 19 OCT 2005
               D QUE L65

     FILE 'CAPLUS, MEDLINE, EMBASE' ENTERED AT 13:00:25 ON 19 OCT 2005
L66            4 DUP REM L57 L65 (2 DUPLICATES REMOVED)
                    ANSWERS '1-4' FROM FILE CAPLUS
               D IBIB ABS HITIND L66 1-4

     FILE 'STNGUIDE' ENTERED AT 13:00:50 ON 19 OCT 2005


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:   17 OCT 2005  HIGHEST RN 865410-76-0
```

DICTIONARY FILE UPDATES: 17 OCT 2005 HIGHEST RN 865410-76-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

FILE CAPLUS

FILE COVERS 1907 - 19 Oct 2005 VOL 143 ISS 17
FILE LAST UPDATED: 18 Oct 2005 (20051018/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Oct 14, 2005 (20051014/UP).

FILE MARPAT
FILE CONTENT: 1988-PRESENT (VOL 143 ISS 15)(20051016/ED)

MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES (COVERAGE TO THESE DATES IS NOT COMPLETE):

US 6916824 12 JUL 2005

DE 1020040544 28 JUL 2005
EP 1555012 20 JUL 2005
JP 2005191426 14 JUL 2005
WO 2005079855 01 SEP 2005

Expanded G-group definition display now available.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

FILE BEILSTEIN
FILE LAST UPDATED ON OCTOBER 10, 2005

FILE COVERS 1771 TO 2005.
FILE CONTAINS 9,363,954 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

****
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *
****

NEW
*** PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.**
*** NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.**

FILE MEDLINE
FILE LAST UPDATED: 18 OCT 2005 (20051018/UP). FILE COVERS 1950 TO DATE.

On December 19, 2004, the 2005 MeSH terms were loaded.

The MEDLINE reload for 2005 is now available. For details enter HELP RLOAD at an arrow promt (=>). See also:

http://www.nlm.nih.gov/mesh/
http://www.nlm.nih.gov/pubs/techbull/nd04/nd04_mesh.html

OLDMEDLINE now back to 1950.

MEDLINE thesauri in the /CN, /CT, and /MN fields incorporate the MeSH 2005 vocabulary.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE EMBASE
FILE COVERS 1974 TO 13 Oct 2005 (20051013/ED)

EMBASE has been reloaded. Enter HELP RLOAD for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.